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BACKGROUND DOCUMENT FOR EPA'S
COMPOSITE MODEL FOR LANDFILLS (EPACML)

Environmental Restoration
Division

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Prepared for

U.S. ENVIRONMENTAL PROTECTION AGENCY
OFFICE OF SOLID WASTE
WASHINGTON D.C. 20460

DISCLAIMER

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ABSTRACT

The Environmental Protection Agency's Composite Landfill Model (EPACML) simulates the movement of contaminants (through the unsaturated and saturated zones) leaching from a hazardous waste landfill. The composite model consists of a steady-state, one-dimensional numerical module that simulates flow in the unsaturated zone. The output from this module, seepage velocity as a function of depth, is used as input by the unsaturated zone transport module. The latter simulates transient, one-dimensional (vertical) transport in the unsaturated zone and includes the effects of longitudinal dispersion, linear adsorption, and first-order decay. Output from the unsaturated zone modules--i.e., contaminant flux at the water table--is used to define the gaussian-source boundary conditions for the transient, semi-analytical saturated zone transport module. The latter includes one-dimensional uniform flow, three-dimensional dispersion, linear adsorption, lumped first-order decay, and dilution due to direct infiltration into the groundwater plume.

The fate and transport of contaminants in the unsaturated and the saturated zones depends on the chemical properties of the contaminants as well as a number of medium- and environment-specific parameters. The uncertainty in these parameters is quantified using the Monte Carlo simulation technique.

The model can be used to back-calculate the allowable concentration of a chemical constituent at the point of release (i.e., below a landfill) such that the receptor well concentration does not exceed a health-based (maximum) threshold level.

This report provides details of the fate and transport modules, the Monte Carlo simulation technique and values of the input parameters that the Agency has compiled based on nationwide surveys of waste disposal facilities.

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SECTION 1

OVERVIEW OF THE LANDFILL MODEL

1.1 INTRODUCTION

This chapter provides an overview of the U.S. Environmental Protection Agency's Composite Model for Landfills (EPACML). The model simulates the fate and transport of contaminants released from a hazardous waste disposal facility into the environment. Release to soil, including the unsaturated and the saturated zone, are included in the model.

The physical scenario being simulated by the model is that of a hazardous waste land disposal facility that releases pollutants into the unsaturated soil, and groundwater. In response to a number of complex physical, chemical, and biological fate and transport processes, the pollutants move in the subsurface environment.

Several factors are considered in the model, including the toxicity, mobility, and persistence of constituents in the waste. The toxicity of a constituent is considered by specifying an allowable health-based concentration level at the point of measurement and back-calculating the maximum acceptable waste leachate concentration that can be released from a land disposal unit (landfill) and not exceed the specified concentration level. The mobility of constituents is considered through incorporation of sorption as a delay mechanism to travel in groundwater. The persistence of organic constituents is incorporated into the groundwater model by considering hydrolysis. Details of the modeling approach were provided in the Federal Register notices of January 14, 1986 (51 FR 1602), June 13, 1986 (51 FR 21648), and August 1, 1988 (53 FR 28892).

1.2 EPACML - AN OVERVIEW

Figure 1-1(a,b) shows a flowchart of the landfill model. The major functions currently performed by this model include:

- Allocation of default values to input parameters/variables.
- Reading of the input data files.
- Echo of input data to output files.
- Generation of random numbers for Monte Carlo simulations.
- Calculation of contaminant degradation rates from hydrolysis rate constants, retardation coefficient, and soil conductivity (from particle diameters) if it is not read in as an input variable.
- Depending on user-selected options:
 - simulation of unsaturated zone flow and transport
 - simulation of saturated zone transport only
 - combinations of the above
- In the Monte Carlo mode, the cumulative frequency distribution (printer plots) and selected percentiles of concentrations at receptors located in the saturated zone are output.
- For each Monte Carlo run, the values of randomly generated input parameters and the computed concentration values can be printed.

The fate and transport of contaminants in the subsurface environment critically depends on a number of unsaturated- and saturated-zone-specific parameters. Typically a number of these parameters exhibit spatial and

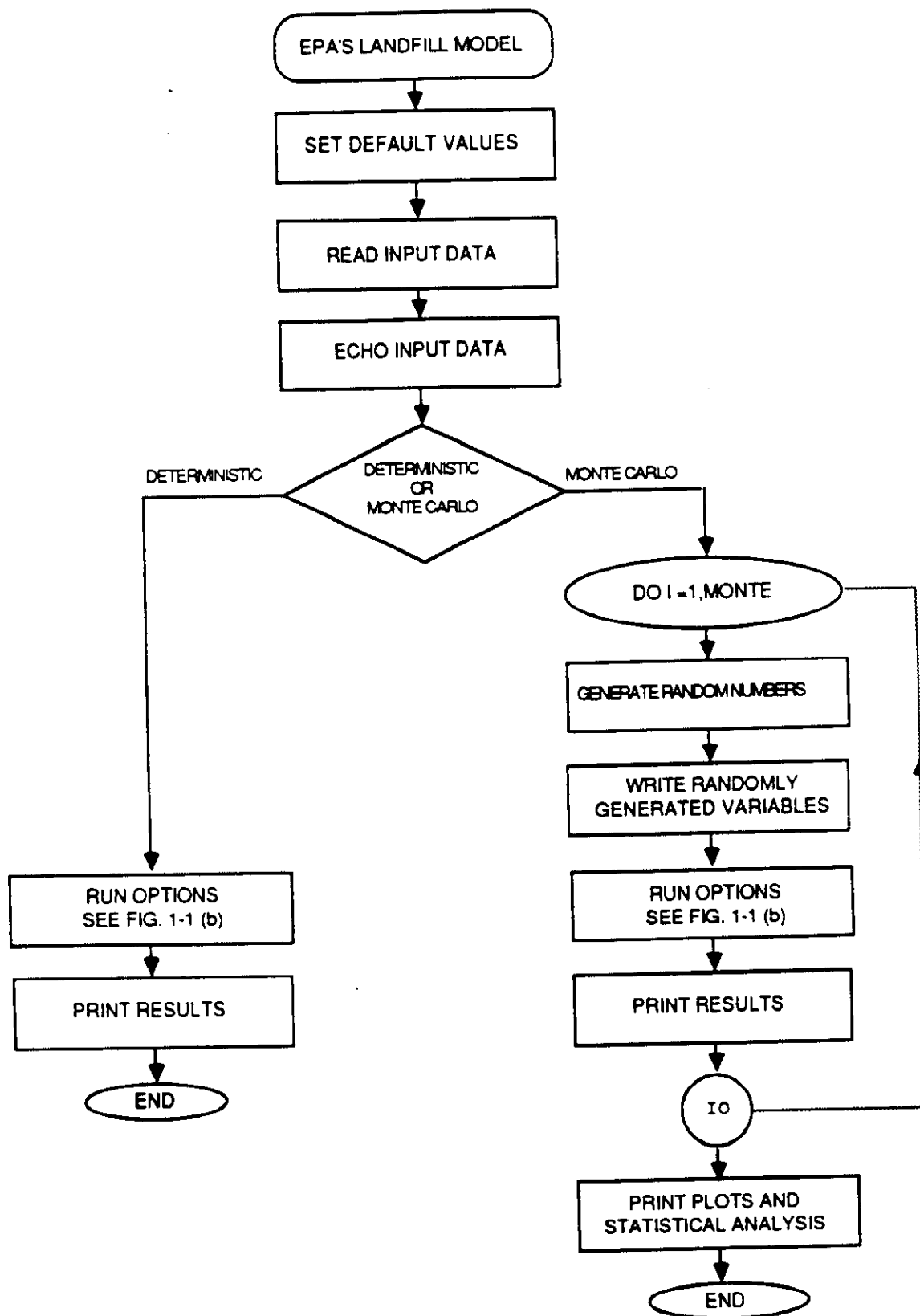


Figure 1-1(a). Flowchart of the EPA's Composite Landfill Model

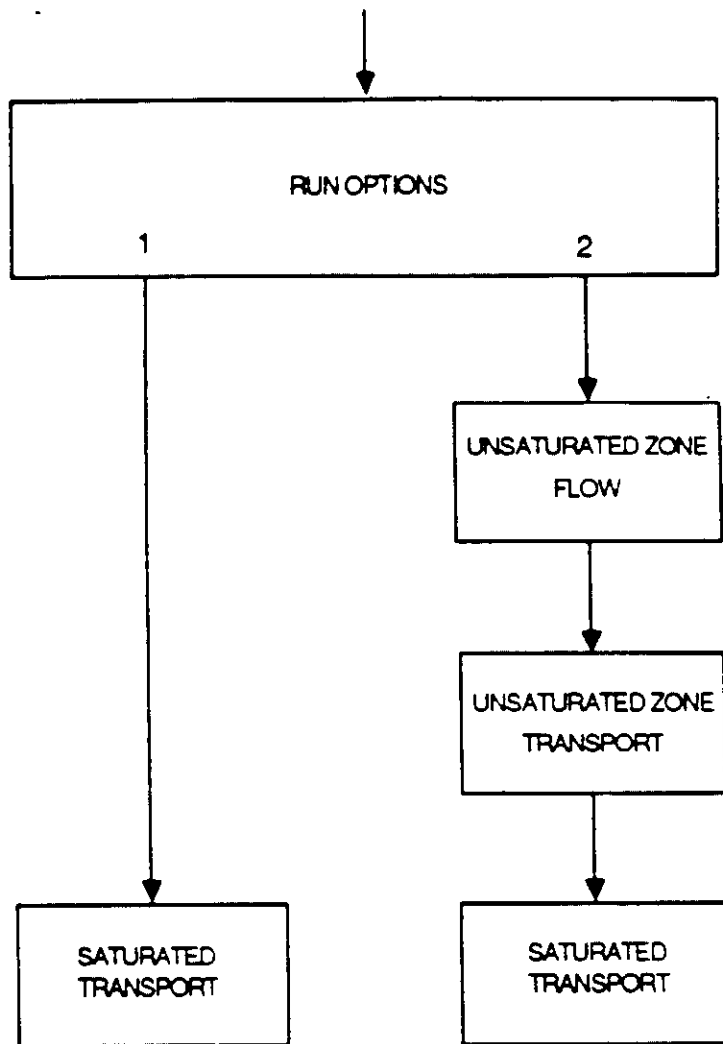


Figure 1-1(b). Flowchart of the Simulation Options In the EPA's Composite Landfill Model

temporal variability as well as variability due to measurement errors. The Landfill Model has the capability to analyze the impact of uncertainty and variability in the model inputs on the model outputs, i.e., concentrations at specified points in the aquifer. The current version treats such variability using the Monte Carlo simulation technique and is discussed in detail in Chapter 5.

Further, since the model would typically be used in the Monte Carlo mode to address the implications of model parameter uncertainties, it was considered necessary to include a post-processing module. This module performs statistical analysis and produces printer plots of the cumulative frequency distributions (CDFs). This uncertainty post-processor also has the capability to combine a number of regional CDFs to yield a composite nationwide CDF of the receptor concentration, as well as to compute confidence bounds for the estimated percentile values.

Finally, the model can be used to 'back-calculate' the concentrations (for steady-state infinite contaminant source case) of the chemical at the source, given a concentration level at a specified distance downgradient from the source. This implies that given a potential point of human exposure and a concentration deemed to be protective of human health and/or the environment, the model can be used to back-calculate the maximum constituent concentration in the leachate immediately beneath or adjacent to the land disposal unit that will ensure that the specified protective level of contaminant concentration is not exceeded at the potential exposure point. The concentration deemed to be protective of human health is termed the RfD (Reference Dose) value.

1.3 REPORT ORGANIZATION

The EPACML model (EPA's Composite Model for Landfills), consists of three modules. These include the unsaturated zone flow and transport module, the saturated zone transport module, and an uncertainty analysis

(Monte Carlo) pre- and post-processing module. Technical details of the saturated zone module are presented in Section 4 of this report. The uncertainty analysis module is discussed in Section 5, and Section 6 contains the default (generic nationwide) values of the data used for the current regulatory implementation of the model. Details of the unsaturated zone flow and transport modules are discussed in Sections 2 and 3 respectively.

SECTION 2

THE UNSATURATED ZONE FLOW MODULE

2.1 INTRODUCTION

In the event that the bottom of the hazardous waste disposal unit is located above the water table, the leachate would migrate through the unsaturated zone and into the saturated zone. A schematic diagram of the leachate migration is shown in Figure 2-1. In such situations it is important to include the unsaturated zone in the analysis of contaminant fate and transport.

This chapter presents details of the semi-analytical unsaturated zone flow module included in the landfill model. Additional details are presented in Huyakorn et al. (1988). The flow module computes the water saturation values within the unsaturated zone which are used by the unsaturated zone transport module to compute seepage velocities. Theoretical details of the flow module and the underlying assumptions and data requirements are presented below.

2.2 GOVERNING EQUATIONS AND SOLUTION TECHNIQUES

The unsaturated zone flow module simulates steady downward flow to the water table. The governing equation is given by Darcy's law:

$$-K_v k_{rw} \left(\frac{\partial \psi}{\partial z} - 1 \right) = I_f \quad (2-1)$$

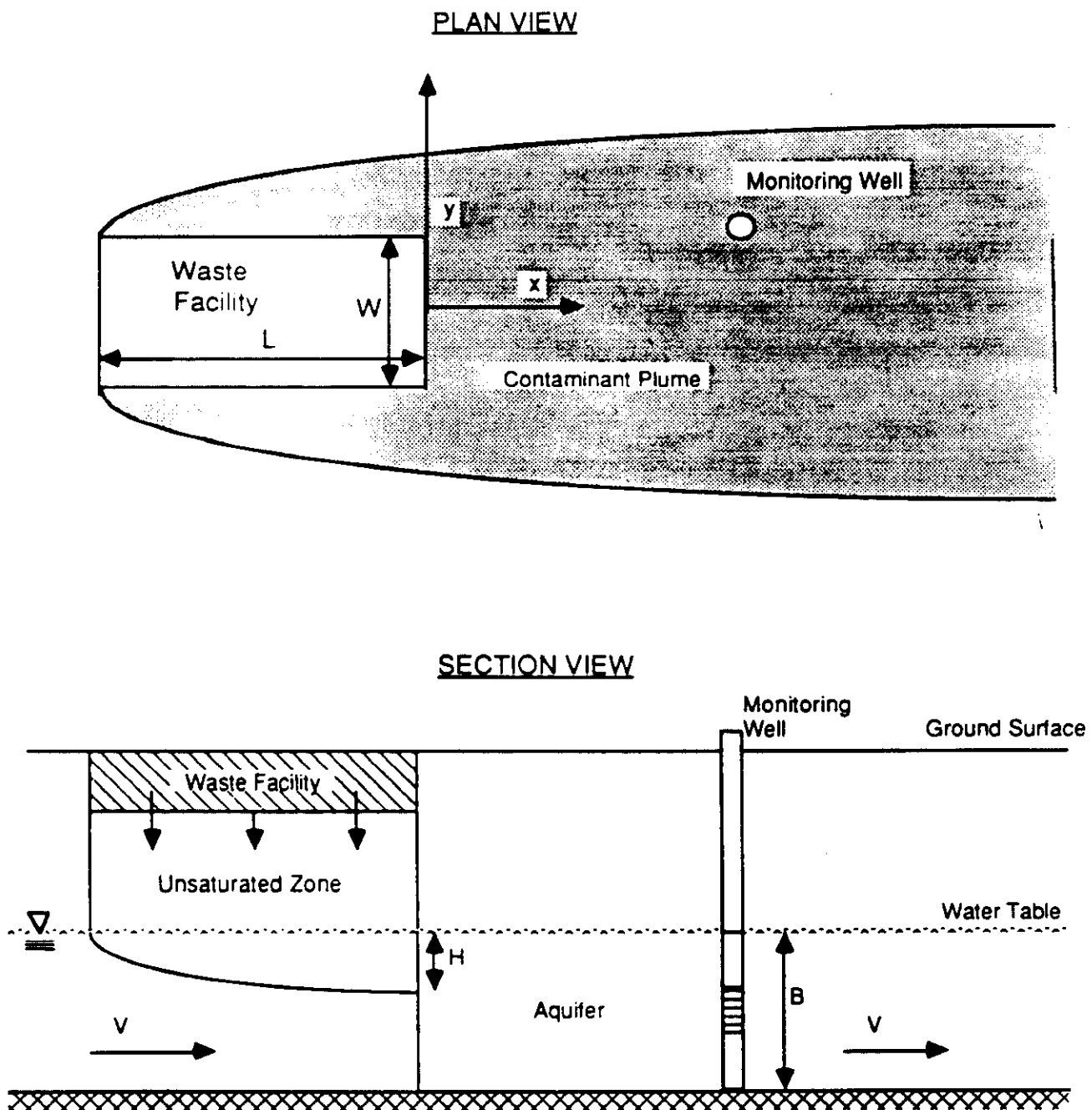


Figure 2-1. A Schematic of the Waste Facility and Leachate Migration Through the Unsaturated and Saturated Zones

where

ψ = the pressure head [m]

z = the depth coordinate which is taken positive downward [m]

K_v = the saturated hydraulic conductivity [m/yr]

k_{rw} = the relative hydraulic conductivity [dimensionless]

I_f = the infiltration rate [m/yr]

The boundary condition at the water table is:

$$\psi(L) = 0 \quad (2-2)$$

where L is the thickness of the unsaturated zone [m].

To solve the above problem, it is necessary to specify the relationships between the relative hydraulic conductivity (k_{rw}) and water saturation (S_w), and between the pressure head (ψ) and water saturation. The following relationships (van Genuchten 1976) are included in the model:

$$k_{rw} = S_e^{1/2} [1 - (1 - S_e^{1/\gamma})^\gamma]^2 \quad (2-3)$$

$$\frac{S_w - S_{wr}}{1 - S_{wr}} = \begin{cases} [1 + (\alpha|\psi - \psi_a|)^B]^{-\gamma} & \text{for } \psi < \psi_a \\ 1 & \text{for } \psi \geq \psi_a \end{cases} \quad (2-4)$$

$$S_e = \frac{(S_w - S_{wr})}{(1 - S_{wr})} \quad (2-5)$$

where

S_{wr} = the residual water saturation [dimensionless]

B, γ = soil-specific parameters [dimensionless]

α = soil-specific parameter [1/m]

ψ_a = the air entry pressure head, which is subsequently assumed zero [m]

S_e = the effective saturation [dimensionless]

Further, the parameters β and γ are related through

$$\gamma = 1 - 1/\beta \quad (2-6)$$

and hence only the parameter β is specified.

Alternatively, the $k_{rw}(S_w)$ relationship presented by Brooks and Corey (1966) may be used. The relationship between the relative hydraulic conductivity and effective saturation is given by:

$$k_{rw} = S_e^n \quad (2-7)$$

Note that the relationship between the saturation water content and the suction pressure head is the same as in Equation 2-4.

As a first step in the solution of Equations 2-1 and 2-2, the soil constitutive relations Equations 2-3 and 2-4 are combined. Using van Genuchten's constitutive equations and assuming $\psi_a = 0$, this leads to the following expression for $k_{rw}(\psi)$:

$$k_{rw} = \begin{cases} 1 & \psi \geq 0 \\ \frac{(1 - (-\alpha\psi)^{\beta-1} [1 + (-\alpha\psi)^\beta]^{1/\beta-1})^2}{[1 + (-\alpha\psi)^\beta]^{(1/2 - 1/2\beta)}} & \psi < 0 \end{cases} \quad (2-8)$$

Next, Equation 2-8 is substituted into Equation 2-1 and the derivative $\frac{\partial \psi}{\partial z}$ replaced by a backward finite difference approximation. This yields, after some rearranging:

$$\frac{K_v}{I_f} \left(\frac{\psi_{z-\Delta z} - \psi_z}{\Delta z} + 1 \right) - 1 = 0, \quad \bar{\psi} \geq 0$$

$$\frac{K_v}{I_f} \frac{(1 - (-\alpha \bar{\psi})^{\beta-1} [1 + (-\alpha \bar{\psi})^\beta]^{1/\beta-1})^2}{[1 + (-\alpha \bar{\psi})^\beta]^{(1/2 - 1/2\beta)}} \left(\frac{\psi_{z-\Delta z} - \psi_z}{\Delta z} + 1 \right) - 1 = 0, \quad \bar{\psi} < 0 \quad (2-9)$$

where $\bar{\psi}$ is the representative pressure head for the soil layer between z and $z - \Delta z$.

If Brooks and Corey's (1966) relationship is used, the expression for relative hydraulic conductivity becomes:

$$k_{rw} = \begin{cases} 1, & \psi \geq 0 \\ (1 + (-\alpha \psi)^\beta)^{-\gamma n}, & \psi < 0 \end{cases} \quad (2-10)$$

Substituting Equation 2-10 into Darcy's law (Equation 2-1), the resulting expression equivalent to Equation 2-9 is:

$$\begin{aligned} \frac{K_v}{I_f} \left(\frac{\psi_{z-\Delta z} - \psi_z}{\Delta z} + 1 \right) - 1 &= 0, & \bar{\psi} \geq 0 \\ \frac{K_v}{I_f} \frac{[1 + (-\alpha \bar{\psi})^\beta]^{-\gamma n}}{[1 + (-\alpha \bar{\psi})^\beta]} \left(\frac{\psi_{z-\Delta z} - \psi_z}{\Delta z} + 1 \right) - 1 &= 0, & \bar{\psi} < 0 \end{aligned} \quad (2-11)$$

In Equations 2-9 and 2-10, $\bar{\psi}$ can be written as a weighted average of ψ_z and $\psi_{z-\Delta z}$:

$$\bar{\psi} = \omega \psi_{z-\Delta z} + (1 - \omega) \psi_z \quad (2-12)$$

where ω is a weighting coefficient ($0 \leq \omega \leq 1$). A value of ω equal to unity was found to give accurate results.

Using Equations 2-9 or 2-11 and 2-12 together with the lower boundary condition Equation 2-2 allows the solution for $\psi_1 = \psi_{L-\Delta z}$. This value

for ψ_1 is then used in place of ψ_2 in Equations 2-9 or 2-11 and 2-12 and the equation is solved for the pressure head at the next desired distance upward from the water table. In this sequential manner, the pressure head at any depth in the unsaturated zone is computed. The Newton-Raphson method is used to solve the nonlinear root-finding problem (Equation 2-9 or 2-10). In the event that the Newton-Raphson method does not converge, the bisection method is used. The latter method is computationally slower but ensures convergence.

After the pressure-head distribution in the unsaturated zone has been found, the corresponding saturation distribution, $S_w(z)$, is computed using Equation 2-4. In principle, the saturation distribution can be found without first solving for $\psi(z)$ by substituting Equation 2-3 or 2-7 rather than Equation 2-8 or 2-10 into Equation 2-1. The disadvantage of this approach is that it becomes more difficult to accommodate nonuniform material properties. Whereas the ψ -profile is continuous in the unsaturated zone, the S_w -profile is discontinuous at the interface of soil layers with contrasting hydraulic properties.

2.3 LIMITATIONS AND ASSUMPTIONS OF THE UNSATURATED ZONE FLOW MODULE

The major assumptions on which the flow module is based include:

- (i) Flow of the fluid phase is considered isothermal, one-dimensional, and governed by Darcy's law.
- (ii) The flow field is considered to be steady.
- (iii) The simultaneous flow of the second phase (i.e., air) can be disregarded.
- (iv) Hysteresis effects are neglected in the specification of the characteristic curves.

2.4 DATA REQUIRED

The data required by the unsaturated zone flow module are listed in Table 2-1. Note that either the van Genuchten's or Brooks and Corey's relationship is required. The current version of the landfill model does not have a source module to estimate the vertical infiltration through the facility and the infiltration is a user-specified variable. The actual values of the data used are presented in Section 6.

Table 2-1. INPUT PARAMETERS REQUIRED FOR UNSATURATED ZONE FLOW MODULE

Parameter	Unit
<u>van Genuchten's Constitutive Relationship</u>	
Soil-specific parameter, β	[dimensionless]
Soil-specific parameter, α	[1/m]
Air entry pressure head, ψ_a	[m]
Residual saturation, S_{wr}	[dimensionless]
<u>Brook and Corey's Constitutive Relationship</u>	
Soil-specific parameter, n	[dimensionless]
Infiltration Rate through the Facility	I_f [m/yr]
Saturated Hydraulic Conductivity of the Soil	K_v [m/yr]
Thickness of the Unsaturated Zone	L [m]

SECTION 3

UNSATURATED ZONE TRANSPORT MODULE

3.1 INTRODUCTION

This section presents the details of the unsaturated zone transport module included in the landfill model. As mentioned above, transport within the unsaturated zone is important only in the event that the bottom of the waste disposal unit is located well above the water table.

This chapter presents the theoretical basis of the unsaturated zone transport module as well as the underlying assumptions. The data requirements for this module are also discussed below.

3.2 GOVERNING EQUATIONS

3.2.1 Unsteady-State Transport

The transport of contaminants within the unsaturated zone is treated as a one-dimensional problem. Important fate and transport mechanisms considered by the module include longitudinal dispersion, linear equilibrium adsorption and first-order decay of the contaminant. With these assumptions, the transport equation can be expressed as:

$$R_v \frac{\partial C}{\partial t} = D_v \frac{\partial^2 C}{\partial z^2} - V_v \frac{\partial C}{\partial z} - \lambda_v R_v C \quad (3-1)$$

where

C = the dissolved-phase contaminant concentration in the unsaturated zone [mg/l]

D_v = the longitudinal dispersion coefficient in the unsaturated zone [m^2/yr]

λ_v = the first-order degradation rate within the unsaturated zone [$1/yr$]

R_v = the unsaturated zone retardation factor

V_v = the steady-state unsaturated zone seepage velocity [m/yr]

t = time [yr]

z = the vertical coordinate which is positive downwards [m]

In Equation 3-1, the retardation factor is computed using:

$$R_v = 1 + \frac{\rho_{bv} K_{dv}}{\theta S_w} \quad (3-2)$$

where

ρ_{bv} = the bulk density of the unsaturated zone [g/cc]

K_{dv} = the contaminant distribution coefficient for the unsaturated zone [cc/g]

θ = the porosity of the unsaturated zone [cc/cc]

S_w = the fractional saturation within the unsaturated zone [cc/cc]

The overall first-order degradation rate, λ_v , includes the effect of both biodegradation and chemical transformation, primarily hydrolysis reactions. The latter is discussed in detail in Section 6.2.

Further in Equation 3-1, the unsaturated zone seepage velocity is computed using:

$$V_v = \frac{I_f}{\theta S_w} \quad (3-3)$$

where I_f is the steady-state infiltration rate within the unsaturated zone. Note that in the landfill model, I_f is assumed to be steady. Also, the saturation, S_w , is computed by the unsaturated zone flow module, as discussed above.

Solution of the above differential equation requires two boundary conditions. The first boundary condition describes the source concentration and may be of the following form:

$$C(0,t) = C_0 \quad (3-4a)$$

or

$$C(0,t) = C_0 \exp(-\lambda t) \quad (3-4b)$$

or

$$C(0,t) = C_0[1 - s(t - T)] \quad (3-4c)$$

where

λ = the source concentration decay rate [1/yr]

$s(t-T)$ = the unit step function with a value of unity for $t > T$ and zero for $t < T$ [t and T are in years]

C_0 = the initial (or steady-state) concentration at the top of the unsaturated zone [mg/l]

Note that Equation 3-4(a) represents a constant source concentration condition, Equation 3-4(b) an exponentially decaying source boundary concentration, and Equation 3-4(c) a finite (constant concentration) pulse source condition. The second boundary condition, which applies at a large distance from the source, is

$$C(\infty,t) = 0 \quad (3-5)$$

The initial condition is

$$C(z,0) = 0 \quad (3-6)$$

The analytical solution for the unsteady-state transport problem has been presented by Marino (1974) and van Genuchten and Alves (1982). Using the constant concentration boundary condition, Equation 3-4(a), the solution can be expressed as:

$$\frac{C}{C_0} = \frac{1}{2} \exp \left[\frac{(V_v - r)z}{2D_v} \right] \operatorname{erfc} \left[\frac{R_v z - r t}{2\sqrt{D_v R_v t}} \right] + \frac{1}{2} \exp \left[\frac{(V_v + r)z}{2D_v} \right] \operatorname{erfc} \left[\frac{R_v z + r t}{2\sqrt{D_v R_v t}} \right] \quad (3-7)$$

Using the exponentially decaying concentration boundary condition, the solution to Equation 3-1 becomes:

$$\begin{aligned} \frac{C}{C_0} = \frac{1}{2} \exp(-\lambda t) \{ & \exp \left[\frac{z(V_v - r_1)}{2D_v} \right] \operatorname{erfc} \left[\frac{R_v z - r_1 t}{2\sqrt{D_v R_v t}} \right] \\ & + \exp \left[\frac{z(V_v + r_1)}{2D_v} \right] \operatorname{erfc} \left[\frac{R_v z + r_1 t}{2\sqrt{D_v R_v t}} \right] \} \end{aligned} \quad (3-8)$$

where r is given by:

$$r = (V_v^2 + 4D_v \lambda_v)^{\frac{1}{2}} \quad (3-9)$$

$$r_1 = [V_v^2 + 4D_v (\lambda_v - \lambda R)]^{\frac{1}{2}}$$

The effect of varying degradation rates, dispersion coefficient and seepage velocity (computed by the flow module) is accounted for by dividing the unsaturated zone into a number of horizontal layers, each one of which is assumed to be homogeneous. This is schematically shown in Figure 3-1.

Equation 3-1 is sequentially solved for each layer. For the first layer, any one of the source boundary conditions, Equation 3-4, can be specified. For the remaining layers, the following source boundary condition, which ensures continuity of concentration, is applied:

$$C_i(x_i, t) = C_{i+1}(0, t) \quad (3-10)$$

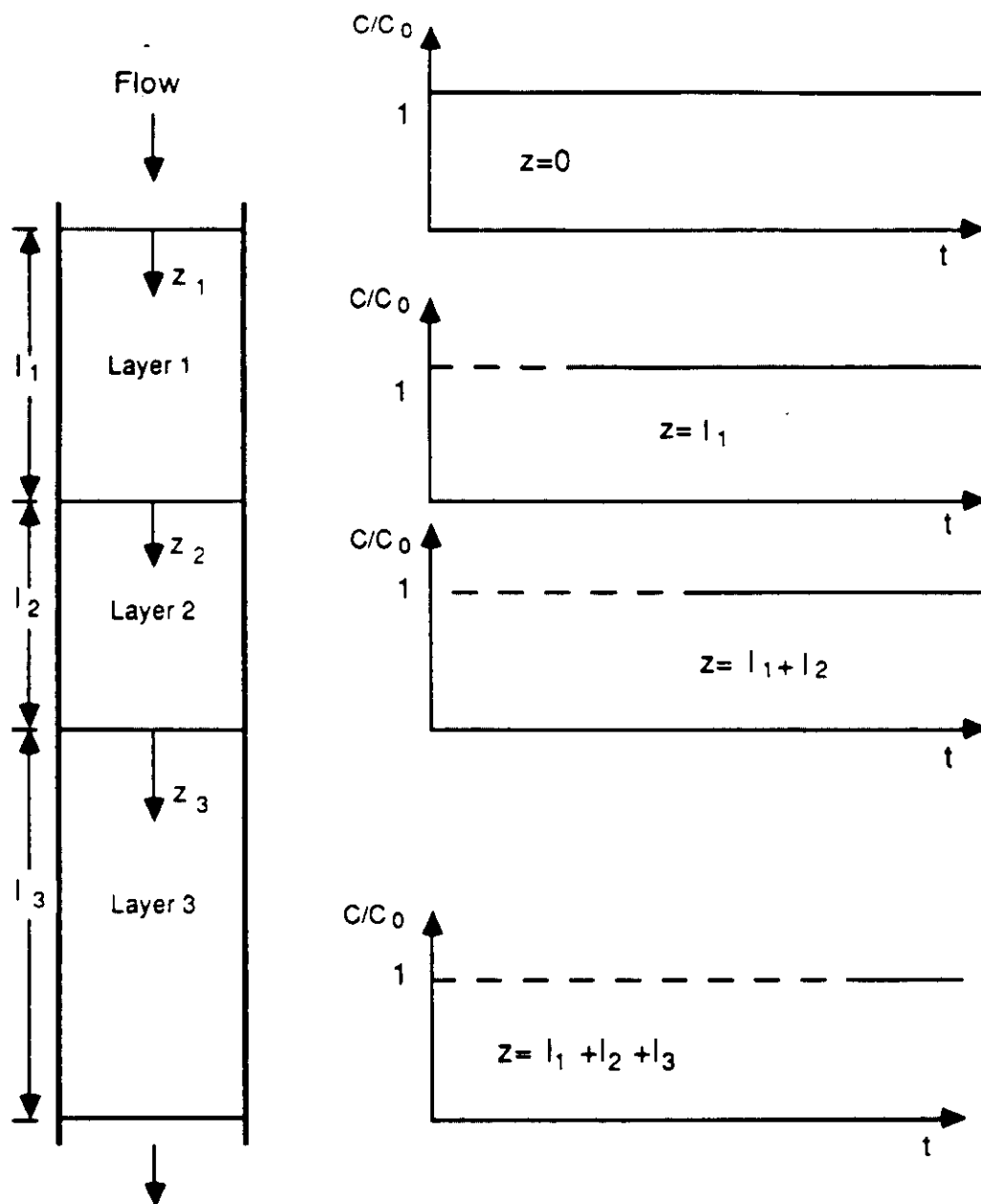


Figure 3-1. A Schematic of Transport Through the Layered Unsaturated Zone

where λ is the thickness of a layer and the subscripts i and $i+1$ refer to successive layers. Equation 3-10 implies that the source concentration at the top of any layer $i+1$ is set equal to the concentration computed at the bottom of the previous layer i . Note that the layers can be of different thickness.

The solution to the layered unsaturated zone is derived using Laplace transform techniques to transform the governing partial differential equation (Equation 3-1) and the boundary conditions to an ordinary differential equation in the Laplace domain. The ordinary differential equation is solved in the Laplace domain and then inverted using either the convolution theorem or the Stehfest algorithm (Stehfest 1970; Moench and Ogata 1981). The latter is a numerical inversion scheme. Both these solution schemes are included in the model. In general, the Stehfest algorithm is computationally faster. However, at very high Peclet numbers there is a possibility that this numerical solution may not converge. For such cases, the convolution integration method may be used. Details of the solution scheme are presented by Shamir and Harleman (1967) and Haderman (1980).

3.2.2 Steady-State Transport

For the case of a steady-state continuous contaminant source, the governing Equation 3-1 can be simplified to yield:

$$\frac{D_v}{R_v} \frac{\partial^2 C}{\partial z^2} - \frac{V_v}{R_v} \frac{\partial C}{\partial z} - \lambda_v C = 0 \quad (3-11)$$

For this case the boundary conditions are:

$$C(z=0) = C_0 \quad (3-12a)$$

$$\frac{\partial C}{\partial z} (z=\infty) = 0 \quad (3-12b)$$

The analytical solution to the above system of equations is:

$$C(z) = C_0 \exp \left\{ \frac{V_v z}{2D_v} - z(\lambda_v R_v / D_v + V_v^2 / 4D_v^2)^{1/2} \right\} \quad (3-13a)$$

or

$$C(z) = C_0 \exp \left\{ \frac{z}{2a_z} - \frac{z}{2a_z} \left(1 + \frac{4\lambda_v a_z R}{V_v} \right)^{1/2} \right\} \quad (3-13b)$$

In the event that dispersion within the unsaturated zone is neglected, the above equation reduces to:

$$\frac{C}{C_0} = \exp \left(\frac{-\lambda_v L}{V_s} \right) \quad (3-14)$$

where L = the depth of the unsaturated zone [m].

For a layered unsaturated zone, Equation 3-14 can be expressed as:

$$\frac{C}{C_0} = \exp \left(-\sum_{i=1}^n \frac{\lambda_{vi} l_i}{V_{vi}} \right) \quad (3-15)$$

where n is the number of homogenous layers within the unsaturated zone.

3.3 LIMITATIONS AND ASSUMPTIONS OF THE UNSATURATED ZONE TRANSPORT MODULE

The major assumptions on which the unsaturated zone transport module is based are:

- (i) The flow field within the unsaturated zone is at a steady state.
- (ii) The seepage velocity as well as other model parameters (dispersion coefficient, partition coefficient, etc.) are uniform in each layer, i.e., each layer is homogeneous and isotropic.
- (iii) Transport is assumed to be strictly one dimensional. Lateral and transverse advection and dispersion are neglected.

- (iv) Adsorption and decay of the solute may be described by a linear equilibrium isotherm and a first-order decay constant, respectively. The daughter products of chemical and biochemical decay are neglected.
- (v) Each layer is approximated as being infinite in thickness. This assumption is valid and introduces negligible errors if the ratio of longitudinal dispersivity to the layer thickness is small ($\ll 1$).

3.4 DATA REQUIRED

Table 3-1 lists the parameters required by the unsaturated zone transport module. The actual values of these parameters are presented in Section 6.

3.4.1 Contaminant Source-Specific Parameters

The unsaturated zone transport module requires three source-specific parameters. These are listed in Table 3-1. Note that the module is linear with respect to the source concentration so that if the source concentration is set to unity, the module computes normalized downgradient well concentrations.

3.4.2 Chemical-Specific Parameters

Table 3-1 lists the four chemical-specific parameters required by the module. These may either be directly input or computed using other parameters as discussed below.

3.4.2.1 The Chemical Transformation Rate--

The chemical decay coefficient is computed using the hydrolysis rate constants as discussed in Section 6.2. The overall decay rate is then computed by adding the biological decay rate to the chemical decay rate.

Table 3-1. INPUT PARAMETERS REQUIRED FOR THE UNSATURATED ZONE TRANSPORT MODULE

Parameter	Unit
<u>Contaminant Source-Specific Parameters</u>	
Source decay constant (for unsteady-state simulation only)	λ [1/yr]
Source concentration at top of unsaturated zone	C_0 [mg/l]
Pulse duration (for unsteady-state simulation only)	T [yr]
<u>Chemical-Specific Parameters</u>	
Chemical transformation rate (computed using hydrolysis rate constant and pH as in the saturated zone transport module)	λ_c [1/yr]
Biodegradation rate	λ_b [1/yr]
Percent organic carbon matter (to compute partition coefficient)	f_{om}
Distribution coefficient	K_{dv} [cc/g]
<u>Unsaturated Zone-Specific Parameters</u>	
Number of layers and thickness of each for transport module	n, z_i [m]
Longitudinal dispersion coefficient	D_v [m ² /yr]
Bulk density of the soil	ρ_{bv} [g/cc]
Porosity of the unsaturated zone	θ [dimensionless]
Seepage velocity (computed by the flow module)	V_s [m/yr]
Temperature of the unsaturated zone layers	T_v [°C]
pH of the unsaturated zone layers	pH

3.4.2.2 The Distribution Coefficient--

In the absence of user-specified values of the distribution coefficient, the latter is computed as the product of the normalized distribution coefficient for organic carbon and the fractional organic carbon content.

3.4.2.3 Percent Organic Carbon Matter--

The value of the fractional organic carbon content is required to compute the distribution coefficient. The former is computed using (Enfield et al. 1982):

$$f_{oc} = \frac{f_{om}}{100 \times 1.724} \quad (3-16)$$

where

f_{oc} = fractional organic carbon content [dimensionless]

f_{om} = percent organic matter content [dimensionless]

3.4.3 Unsaturated Zone-Specific Parameters

Table 3-1 lists the unsaturated zone specific transport parameters. Of these, the seepage velocity is computed using Equation 3-3, with the saturation values computed by the unsaturated zone flow module. All other values are user-specified input except for the longitudinal dispersion coefficient, which is computed as discussed below.

3.4.3.1 Longitudinal Dispersion Coefficient--

The longitudinal dispersion values are computed using the relationship:

$$D_v = \alpha_v V_v \quad (3-17)$$

where

D_v = the longitudinal dispersion coefficient [m^2/yr]

V_v = the seepage velocity in the unsaturated zone [m/yr]

α_v = the longitudinal dispersivity [m]

The dispersivity values used in the models are based on an analysis of the data presented by Gelhar et al. (1985) shown in Table 3-2. Using regression analysis, the following relation was developed:

$$\alpha_v = .02 + .022L, \quad R^2 = 66\% \quad (3-18)$$

where L is the depth of the unsaturated zone. To avoid excessively high values of dispersivity for deep unsaturated zones, a maximum dispersivity of 1.0 m is used. Thus, for all depths greater than 44.5 m, α_v will be set equal to 1.0 m.

Table 3-2. COMPILATION OF FIELD DISPERSIVITY VALUES (GELHAR ET AL. 1985)

Author	Type of Experiment	Vertical Scale of Experiment [m]	Longitudinal Dispersivity α_v [m]
Yule and Gardner (1978)	Laboratory	0.23	0.0022
Hildebrand and Himmelblau (1977)	Laboratory	0.79	0.0018
Kirda et al. (1973)	Laboratory	0.60	0.004
Gaudet et al. (1977)	Laboratory	0.94	0.01
Brissaud et al. (1983)	Field	1.00	0.0011, 0.002
Warrick et al. (1971)	Field	1.20	0.027
Van de Pol et al. (1977)	Field	1.50	0.0941
Biggar and Nielsen (1976)	Field	1.83	0.05
Kies (1981)	Field	2.00	0.168
Jury et al. (1982)	Field	2.00	0.0945
Andersen et al. (1968)	Field	20.00	0.70
Oakes (1977)	Field	20.00	0.20

SECTION 4

THE SATURATED ZONE MODULE

4.1 INTRODUCTION

This chapter presents details of the module used to simulate contaminant fate and transport within the saturated porous zone. Recall that the contaminant can enter the saturated formation by direct leaching from the waste disposal unit (in the absence of an unsaturated zone) or by percolation through the unsaturated zone. The composite model allows the user to specify either of the above options. Note that in both cases the governing equations, and hence the semi-analytical solution for transport in the saturated zone, is the same.

The following sections describe the governing equations, boundary and initial conditions, model limitations, and the parameters required to solve the equations.

4.2 GOVERNING EQUATIONS

The three-dimensional solute transport equation on which the model is based can be written as:

$$D_x \frac{\partial^2 C}{\partial x^2} + D_y \frac{\partial^2 C}{\partial y^2} + D_z \frac{\partial^2 C}{\partial z^2} - V_s \frac{\partial C}{\partial x} = R_s \frac{\partial C}{\partial t} + R_s \lambda_s C + R_s \frac{qC}{B} \quad (4-1)$$

where:

x, y, z = spatial coordinates in the longitudinal, lateral and vertical directions, respectively [m]

C = dissolved concentration of chemical [mg/l, g/m³]

D_x, D_y, D_z = dispersion coefficients in the x, y and z directions, respectively [m²/yr]

V_s = one-dimensional, uniform seepage velocity in the x direction [m/yr]

R_s = retardation factor in the saturated zone [dimensionless]

t = elapsed time [yr]

λ_s = effective first-order decay coefficient in the saturated zone [1/yr]

q = net recharge outside the facility percolating directly into and diluting the contaminant plume [m/yr]

B = the thickness of the saturated zone [m]

In Equation 4-1, the retardation factor and the effective decay coefficient are defined as:

$$R_s = 1 + \frac{\rho_b K_d}{\theta} \quad (4-2)$$

and

$$\lambda_s = \frac{\lambda_1 \theta + \lambda_2 \rho_b K_d}{\theta + \rho_b K_d} + \lambda_b \quad (4-3)$$

where:

ρ_b = bulk density of the porous media [g/cc]

K_d = distribution coefficient [cc/g]

θ = effective porosity for the saturated zone [cc/cc]

λ_1 = first-order decay constant for dissolved phase [1/yr]

λ_2 = first-order decay constant for the sorbed phase [1/yr]

λ_b = first-order lumped biodegradation rate in the saturated zone [1/yr]

The flow domain is regarded as semi-infinite in the x direction ($0 \leq x \leq \infty$), infinite in the y-direction ($-\infty \leq y \leq \infty$) and finite in the z-direction ($0 \leq z \leq B$).

Solution of Equation 4-1 requires initial and two-boundary conditions in the x, y, and z directions. At the source (downstream edge of the waste disposal unit) the contaminant concentration is assumed to be a gaussian distribution in the lateral direction and uniform over the vertical mixing or penetration depth, H. A schematic description of the flow domain and the source boundary condition is shown in Figure 4-1. Mathematically, the above-stated assumptions can be expressed as:

$$C(x, y, z, 0) = 0 \quad (4-4a)$$

$$C(0, y, z, t) = \begin{cases} C_0 \exp[-y^2/(2\sigma^2)], & 0 \leq z \leq H \\ 0, & H < z \leq B \end{cases} \quad (4-4b)$$

$$C(\infty, y, z, t) = 0 \quad (4-4c)$$

$$C(x, \pm\infty, z, t) = 0 \quad (4-4d)$$

$$\frac{\partial C}{\partial z}(x, y, 0, t) = 0 \quad (4-4e)$$

$$\frac{\partial C}{\partial z}(x, y, B, t) = 0 \quad (4-4f)$$

In Equation 4-4b, the source boundary condition, C_0 [mg/l], is the maximum dissolved concentration of the solute at the source and occurs at the center of the gaussian distribution. Also, the standard deviation, σ , is a measure of the width of the source. Further note that Equations 4-4e and 4-4f imply that there is zero flux of contaminant at $z = 0$ and $z = B$.

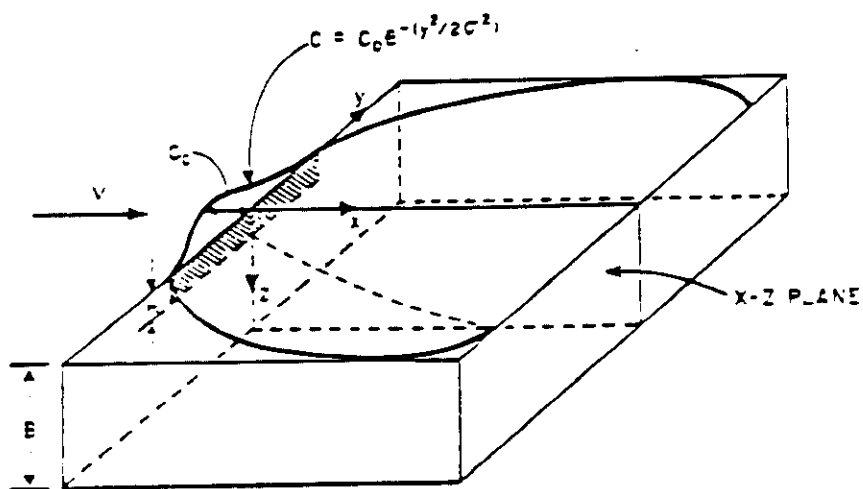


Figure 4-1. A Schematic Diagram of the Source Boundary Conditions for the Saturated Zone Transport Module

Huyakorn et al. (1987) have presented analytical solutions for the system of Equations 4-1 to 4-4. The general solution can be expressed as:

$$C(x, y, z, t) = \frac{H}{B} C_f(x, y, t) + \Delta C_p(x, y, z, t) \quad (4-5)$$

where C_f and ΔC_p are functions given by:

$$C_f(x, y, t) = \xi \int_0^t F(x, y, \tau) \exp(-\eta \tau) d\tau \quad (4-6)$$

$$\begin{aligned} \Delta C_p(x, y, z, t) = & \frac{2\xi}{\pi} \sum_{n=1}^{\infty} \frac{1}{n} \cos\left(\frac{n\pi z}{B}\right) \sin\left(\frac{n\pi H}{B}\right) \\ & \cdot \int_0^t F(x, y, \tau) \exp(-\eta_n \tau) d\tau \end{aligned} \quad (4-7)$$

in which

$$\begin{aligned} F(x, y, \tau) = & \frac{1}{\tau^{3/2} (2\sigma^2 + 4D_y^* \tau)^{1/2}} \\ & \cdot \exp\left(-\frac{x^2}{4D_x^* \tau} - \frac{y^2}{4D_y^* \tau + 2\sigma^2}\right) \end{aligned} \quad (4-8a)$$

$$\xi = \frac{C_0 \sigma x}{(2\pi D_x^*)^{1/2}} \exp\left(\frac{V_s^* x}{2D_x^*}\right) \quad (4-8b)$$

$$\eta = \frac{V_s^{*2}}{4D_x^*} + \lambda \quad (4-8c)$$

$$B_n = \eta + \frac{n^2 \pi^2 D_z^*}{B^2} \quad (4-8d)$$

where:

D_x^* , D_y^* , and D_z^* = the retarded dispersion coefficients (D_x/R_s , D_y/R_s , D_z/R_s) in the x, y and z direction

V_s^* = the retarded solute (seepage) velocity [$V_s^* = V_s/R_s$]

τ = the variable of integration

Note that in the event that $H = B$, i.e., the source fully penetrates the saturated formation, $\Delta C_p = 0$ in Eq. 4.5. At any distance, x , from the source, maximum contaminant concentration would occur at the centerline of the plume and can be represented as:

$$C(x, 0, 0, t) = \frac{H}{B} C_f(x, 0, t) + \Delta C_p(x, 0, 0, t) \quad (4-9)$$

where $C_f(x, 0, t)$ and $\Delta C_p(x, 0, 0, t)$ are given by Equations 4-6 and 4-7 with arguments y and z set equal to zero, and the function $F(x, 0, \tau)$ defined as:

$$F(x, 0, \tau) = \frac{\exp(-x^2/4D_x^*\tau)}{\tau^{3/2} (2\sigma^2 + 4D_y^*\tau)^{1/2}} \quad (4-10)$$

As t approaches infinity, a steady-state condition is reached. The steady-state concentration along the plume centerline can be expressed as:

$$C^*(x, 0, 0) = \frac{H}{B} C_f^*(x, 0) + \Delta C_p^*(x, 0, 0) \quad (4-11)$$

where:

$$C_f^*(x, 0) = \xi^* \int_0^{\infty} \exp \left[-\frac{\sigma^2 u^2}{2} - x \left(\frac{u^2 D_x^*}{D_x^*} + \frac{n}{D_x^*} \right) \right]^{1/2} du \quad (4-12a)$$

$$\Delta C_p^*(x, 0, 0) = \frac{2\xi^*}{\pi} \sum_{n=1}^{\infty} \frac{1}{n} \sin \left(\frac{n\pi H}{B} \right)$$

$$\int_0^{\infty} \exp \left[-\frac{c^2 u^2}{2} - x \left(\frac{u^2 D_x^*}{D_x^*} + \frac{n}{D_x^*} \right) \right]^{1/2} du \quad (4-12b)$$

$$\xi^* = \frac{2C_{0\sigma}}{(2\pi)^{1/2}} \exp \left(\frac{V_s^* x}{2D_x^*} \right) \quad (4-12c)$$

The above solution for the transient state, i.e., Equations 4-5 to 4-8d, was earlier programmed in FORTRAN 77 in the code named EPATMOD. Similarly, the steady-state solution, Equations 4-11 and 4-12, has been programmed in the code named EPASMOD. In these codes, the integrals in Equation 4-7 and Equation 4-12 are computed numerically using the Gauss-Quadrature scheme (Carnahan et al. 1969). Note that for large time, t , EPATMOD yields the steady-state solution that is identically equal to EPASMOD. However, the code EPASMOD is significantly faster than EPATMOD and should be used for steady-state computations. Finally, note that the model uses the principle of superposition, to compute the plume concentration for a pulse source, i.e., a contaminant source of finite duration, T_s . Both these codes have been incorporated into the composite code, EPACML, and constitute the saturated zone transport module of this code.

The concentrations computed by the saturated zone model at a down-gradient location (e.g., receptor well) can be used in a back calculation

mode as explained in Section 5.6 to estimate the maximum allowable leachate concentration at the waste disposal facility.

4.3 ASSUMPTIONS AND LIMITATIONS OF THE SATURATED ZONE TRANSPORT MODULE

Following are the list of assumptions inherent in the saturated zone transport module:

- i) The saturated, porous medium properties are isotropic and homogeneous. The module cannot be used to simulate transport in fractured media unless the fractured medium is represented as an equivalent porous formation.
- ii) The groundwater flow velocity is steady and uniform. This implies that the recharge through the facility and into the groundwater plume is small compared to the natural (regional) flow.
- iii) Contaminant degradation/transformation follows the first-order rate law and is restricted to biodegradation and hydrolysis. The latter is a second-order process from which the first-order rate is obtained using existing environmental conditions, i.e., pH. This assumption is conservative since it neglects degradation due to other mechanisms such as oxidation, reduction, etc. Further, the by-products of degradation are neglected.
- iv) Contaminant sorption follows a linear adsorption isotherm. Adsorption takes place instantaneously and the adsorbed phase is in local equilibrium.
- v) Assumptions regarding the source boundary conditions and the extent of the formation have been discussed in Section 4.2.

4.4 COUPLING OF THE UNSATURATED AND THE SATURATED ZONE MODULES

In the event that the transport of contaminants through the unsaturated and the saturated zones are considered, an important requirement is that the principle of conservation of mass be satisfied, i.e., the mass flux that leaches out of the facility (in the absence of an unsaturated zone or from the bottom of the unsaturated zone) be equal to the mass flux that enters the saturated zone. This mass flux consists of the sum of advective and dispersive mass fluxes.

4.4.1 Steady-State Coupling

The mass that leaches out of the facility can be expressed as:

$$M_L = A_w I_f C_L \quad (4-13)$$

where:

M_L = the mass that leaches out of the facility [g/yr]

A_w = the area of the facility [m^2]

I_f = infiltration rate through the facility [m/yr]

C_L = concentration in the leachate from the facility [g/m^3] if attenuation within the unsaturated zone is neglected or the unsaturated zone is absent. Alternatively, C_L is the estimated concentration at the bottom of the unsaturated zone.

The mass flux that is advected into the saturated zone is calculated by integrating the source concentration in the y direction from $-\infty$ to $+\infty$ and over the depth $z = 0$ to $z = H$. Thus the mass flux advected into the aquifer is:

$$M_a = \int_{z=0}^H \int_{y=-\infty}^{+\infty} C(x=0, y, z) V_s \theta \, dy \, dz \quad (4-14)$$

where:

M_a = mass flux advected into the aquifer [g/yr]

$C(x = 0, y, z)$ = concentration as a function of y and z at the source
[g/m³, mg/l] as expressed by Eq. 4-4b

V_s = the seepage velocity in the saturated zone [m/yr]

θ = effective porosity of the saturated zone [cc/cc]

Similarly, the mass flux that enters the saturated zone due to dispersion can be expressed as:

$$M_d = \int_{z=0}^H \int_{y=-\infty}^{+\infty} \theta D \left. \frac{\partial C}{\partial x} \right|_{x=0} dy dz \quad (4-15)$$

Integrating Equation 4-14, with C_0 assumed uniform over the source depth H , yields:

$$M_a = (2\pi)^{1/2} \sigma V_s \theta H C_0 \quad (4-16)$$

Ungs (1987) (attached as Appendix A) has evaluated the integral in Equation 4-15 to yield:

$$M_d = (2\pi)^{1/2} \sigma V_s \theta H C_0 \left[-\frac{1}{2} + \frac{1}{2} \left(1 + \frac{4 \lambda_s R_s D_x}{V_s^2} \right)^{1/2} \right] \quad (4-17)$$

where:

λ_s = the overall first-order decay coefficient [1/yr]

R_s = the linear retardation factor [dimensionless]

D_x = the longitudinal dispersion coefficient [m²/yr]

Note that in the event that $D_x = 0$, the dispersive flux, M_d , is zero. Thus the total flux into the saturated zone is given by the sum of advective (Equation 4-16) and dispersive (Equation 4-17) fluxes:

$$M_T = (2\pi)^{1/2} \sigma V_s \theta H C_0 \epsilon_D \quad (4-18)$$

where:

$$\epsilon_D = \left[\frac{1}{2} + \frac{1}{2} \left(1 + \frac{4 \lambda_s R_s D_x}{V_s^2} \right)^{\frac{1}{2}} \right] \quad (4-19)$$

Note that if ϵ_D is set equal to unity, it implies that the dispersive flux is neglected.

Equating Equations 4-13 and 4-19 yields the following expression of the mass balance:

$$A_w I_f C_L = (2 \pi)^{\frac{1}{2}} \sigma V_s \theta H C_0 \epsilon_D \quad (4-20)$$

The above equation is used to couple the unsaturated and the saturated zone models under steady-state conditions.

4.4.2 Unsteady-State Coupling

For the case of unsteady-state transport in the unsaturated zone, the mass flux at the water table varies in time, and the above approach for coupling the unsaturated and the saturated zone is no longer valid. In the unsteady state, concentrations in the saturated zone are determined using the convolution integration approach that superimposes the effects of source changes over time as follows:

$$C(x,y,z,t) = \int_0^t \left. \frac{\partial C^*}{\partial \tau} \right|_{\tau} f(x,y,z,t - \tau) d\tau \quad (4-21)$$

where:

$C^*(t)$ = the concentration at the water table at time t [mg/l]

$f(x,y,z,t)$ = the normalized (with respect to source concentration)
solution of the saturated zone analytical solution
[mg/l]

In Equation 4-21, the value of $f(x,y,z,t)$ is the solution to the saturated zone transport equation with the gaussian source boundary condition. In the computer code program, the above integral is numerically evaluated using the trapezoidal rule.

4.5 PARAMETERS REQUIRED BY THE SATURATED ZONE TRANSPORT MODULE

Table 4-1 lists the input parameters required to compute the contaminant concentrations in the saturated zone. These parameters can be classified into the following four groups:

- (1) Contaminant source-specific parameters
- (2) Aquifer-specific parameters
- (3) Chemical-specific parameters
- (4) Receptor well location-specific parameters

Important qualitative and quantitative aspects of each of these input parameters are discussed below.

Note that in the event that values of the parameters listed in Table 4-1 are not available, the EPACML code includes the option of deriving these using other variables (presented in Table 4-2) and using a set of empirical, semi-empirical or exact relationships as discussed below. The specific parameter values and the empirical relationships used while implementing the code for the current regulation are described in Section 6.

4.5.1 Source-Specific Parameters

For steady-state analysis, the model requires three source-specific parameters. These parameters are estimated based on the mass balance Equation 4-20 and consideration of other physical/empirical information as explained below.

Table 4-1. INPUT PARAMETERS REQUIRED FOR THE SATURATED ZONE TRANSPORT MODULE*

Parameter	Unit
<u>Contaminant Source-Specific Parameters</u>	
<u>Steady-State</u>	
Leachate concentration at the waste facility	C_0 [mg/l, g/m ³]
Standard deviation of the source	σ [m]
Thickness of gaussian source	H [m]
<u>Unsteady State (additional parameter)</u>	
Duration of the pulse	T_s [yr]
<u>Aquifer-Specific Parameters</u>	
Porosity	ϕ [cc/cc]
Bulk density	ρ_b [g/cc]
Thickness of the aquifer	B [m]
Seepage velocity	V_s [m/yr]
Longitudinal dispersion coefficient	D_x [m ² /yr]
Lateral dispersion coefficient	D_y [m ² /yr]
Vertical dispersion coefficient	D_z [m ² /yr]
Aquifer temperature	T [°C]
Recharge rate into the plume	q [m/yr]
<u>Chemical-Specific Parameters</u>	
Effective first-order decay coefficient	λ_s [1/yr]
Distribution coefficient	K_d [cc/g]
Biodegradation rate	λ_b [1/yr]

Table 4-1. INPUT PARAMETERS REQUIRED FOR THE SATURATED ZONE TRANSPORT MODULE* (concluded)

Parameter	Unit
<u>Receptor Well Location-Specific Parameters</u>	
Coordinates with respect to the source	x_r, y_r, z_r [m]
Time value at which concentration is required	t_r [yr]

*A few of the parameters are derived from variables shown in Table 4-2.

Table 4-2. ADDITIONAL DATA REQUIRED TO COMPUTE INPUT PARAMETERS FOR THE SATURATED ZONE TRANSPORT MODULE

Parameter	Unit
<u>Input Variables to Compute Source-Specific Parameters</u>	
Area of the land disposal facility	A_w [m ²]
Infiltration rate through the facility	I_f [m/yr]
<u>Input Variables to Compute Aquifer-Specific Parameters</u>	
Mean particle diameter of the porous medium	d [cm]
The hydraulic gradient	S [m/m]
Longitudinal dispersivity	α_L [m]
Transverse dispersivity	α_T [m]
Vertical dispersivity	α_V [m]
<u>Input Variables to Compute Chemical-Specific Parameters</u>	
Reference temperature	T_r [°C]
Second-order acid-catalysis hydrolysis rate constant at reference temperature	K_a^r [L/mole-yr]
Second-order base-catalysis hydrolysis rate constant at reference temperature	K_b^r [L/mole-yr]
Neutral hydrolysis rate constant at reference temperature	K_n^r [1/yr]
pH of the aquifer	pH [log 10 mole/L]
Normalized distribution coefficient for organic carbon	K_{oc} [mL/g]
Fractional organic carbon content	f_{oc} [dimensionless]
<u>Input Variables to Compute Receptor Well Location-Specific Parameters</u>	
Radial distance to well	R [m]
Angle to the well location	ψ [degrees]

4.5.1.1 Depth of Penetration of Source--

Infiltration of water through the facility results in the development of a plume below the facility. This is shown in Figure 4-2. The thickness of this plume depends on the vertical dispersivity of the media. An estimate of 'H' can thus be obtained using the following relationship:

$$H = (2\alpha_v L)^{\frac{1}{2}} + B(1 - \exp(-\frac{LI_f}{V_s \theta B})) \quad (4-22)$$

where:

α_v = the vertical dispersivity [m]

L = the length scale of the facility--i.e., the dimension of the facility parallel to the flow direction [m] (if L is not known, an estimate can be obtained from Equation 4-23)

B = the thickness of the saturated zone [m]

In Equation 4-22 the first term represents the thickness of the plume due to vertical dispersion and the second term represents the thickness of the plume due to the vertical velocity below the facility resulting from infiltration. The detailed derivation of the second term is presented in the attached document (Appendix B). While implementing this alternative, it is necessary to specify that in the event that the computed value of H is greater than B, the thickness of the source, H, is set equal to B.

If L is not known, an estimate can be obtained by taking the square root of the area, i.e.,

$$L = (A_w)^{\frac{1}{2}} \quad (4-23)$$

The above assumes that the waste disposal facility has a square shape.

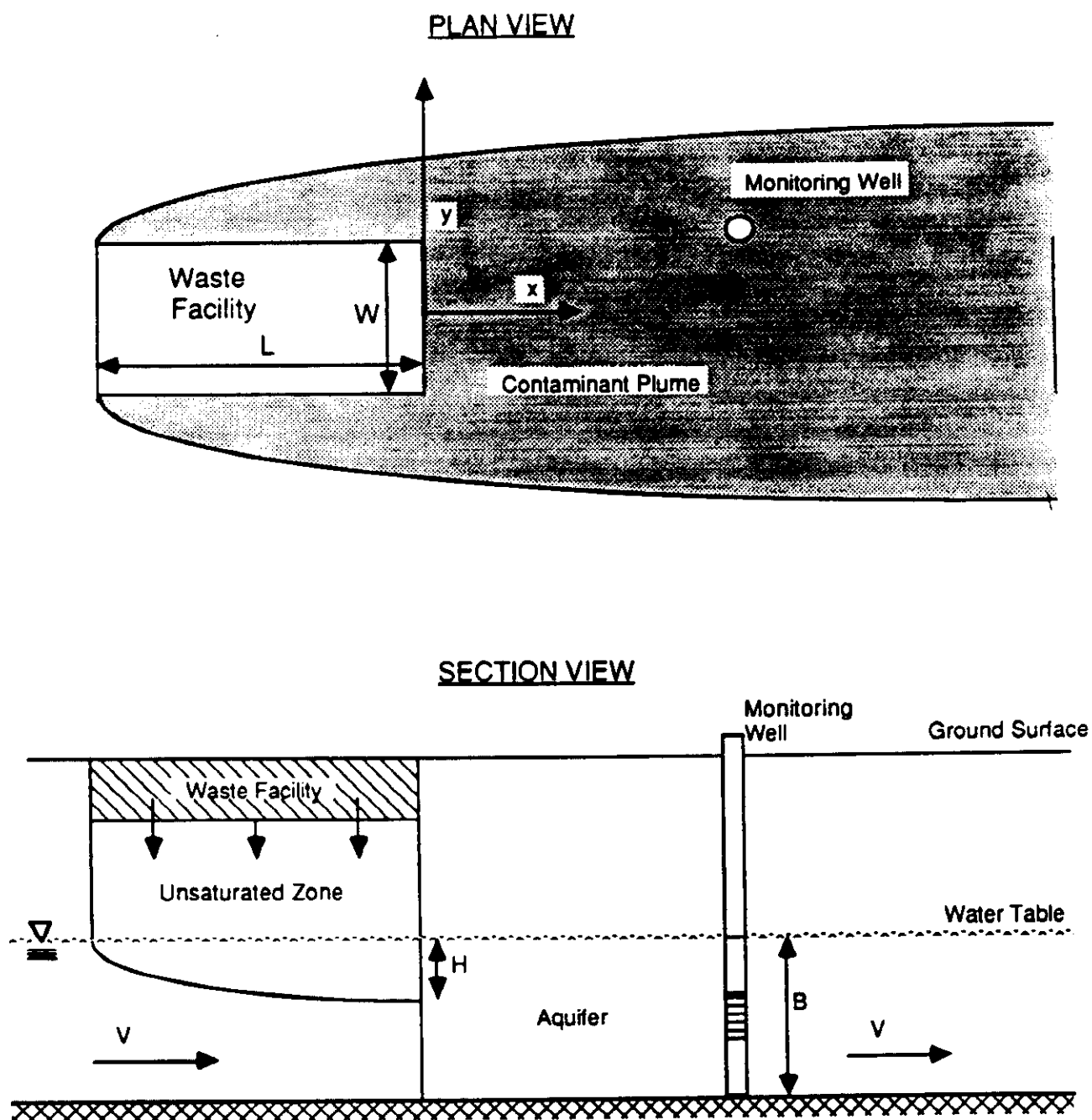


Figure 4-2. A Schematic of the Waste Facility and Leachate Migration Through the Unsaturated and Saturated Zones

4.5.1.2 The Spread of the Gaussian Source--

The standard deviation of the gaussian source is a measure of the spread of the source and can be estimated as:

$$\sigma = W/6 \quad (4-24)$$

where:

W = the width scale of the facility--i.e., the dimension of the facility orthogonal to the groundwater flow direction [m]

Dividing by 6 implies that 99.86 percent of the area under the gaussian source is flanked by the width of the facility. Note that if the orientation of the facility with respect to the groundwater flow direction is not known, then a measure of width of the facility can be obtained by taking the square root of the area, as in Equation 4-23.

4.5.1.3 Maximum Source Concentration--

Having obtained both H and σ (using Equations 4-22 and 4-24, respectively) based on physical considerations, the mass balance equation can be used to compute C_0 , i.e.,

$$C_0 = \frac{A_w I_f}{(2\pi)^{1/2} V_s \theta H \sigma z_D} C_i \quad (4-25)$$

or

$$C_0 = (NMF) C_i \quad (4-26)$$

In Equation 4-26 the factor NMF can be thought of as representing a near-field dilution effect or the effect of mixing below the facility; this factor, based on purely physical considerations, should be less than or at most equal to unity to ensure that $C_0 \leq C_i$. Note that the use of

Equation 4-26 presents the problem of estimating C_g . A conservative maximum value of C_g would be the solubility of the contaminant in water.

4.5.1.4 Other Parameters Required--

Computation of the source-specific parameters using the above method, Equations 4-22, 4-24, and 4-26, requires knowledge of the area of the facility; the infiltration rate through the facility; aquifer-specific variables including seepage velocity, porosity, longitudinal dispersivity and depth of the aquifer; and chemical-specific adsorption coefficient. These are discussed in the following section.

4.5.2 Aquifer-Specific Parameters

The model requires nine aquifer-specific parameters listed in Table 4-1. These can be input directly or computed using the variables listed in Table 4-2 and the relationships presented below.

4.5.2.1 Porosity--

In the absence of user-specified distribution for porosity, it can be calculated from the particle diameter using the following empirical relationship (Federal Register Vol. 51, No. 9, pp. 1649, 1986):

$$\theta = 0.261 - 0.0385 \ln(d) \quad (4-27)$$

where d = the mean particle diameter [cm].

4.5.2.2 Bulk Density--

The soil bulk density directly influences the retardation of solutes and is related to the soil structure. An exact relationship between the soil porosity, particle density and the bulk density can be derived (Freeze and Cherry 1979). Assuming the particle density to be 2.65 g/cc, this relationship can be expressed as:

$$\rho_b = 2.65(1 - \theta) \quad (4-28)$$

where ρ_b = the bulk density of the soil [g/cc].

4.5.2.3 Seepage Velocity--

The seepage velocity is related to the aquifer properties through the Darcy's law. Assuming a uniform, saturated porous medium, the magnitude of the seepage velocity can be expressed as:

$$V_s = \frac{KS}{\theta} \quad (4-29)$$

where:

K = the hydraulic conductivity of the formation [m/yr]

S = the hydraulic gradient [m/m]

Note that in general, the hydraulic gradient is a function of the local topography, groundwater recharge volume and location, and the volume and location of groundwater withdrawals. Further, it may also be related to the porous media properties.

4.5.2.4 Hydraulic Conductivity--

In the absence of site-specific measurements, the hydraulic conductivity can be calculated using approximate functional relationships. One such relationship included in the model, the Karman-Cozeny equation (Bear 1979), can be expressed as:

$$K = \frac{\rho g}{\mu} \frac{\theta^3}{(1-\theta)^2} \frac{d^2}{1.8} \quad (4-30)$$

where:

K = the hydraulic conductivity [cm/s]
 ρ = the density of water [kg/m³]
 g = acceleration due to gravity [m/s²]
 μ = the dynamic viscosity of water [N-s/m²]
 d = mean particle diameter [cm]

In Equation 4-30 the constant 1.8 includes a unit conversion factor. Both the density of water (ρ) and the dynamic viscosity of water are functions of temperature and are computed using regression equations presented in CRC (1981). Note that at 15°C, the value of [$\rho g / 1.8 \mu$] is about 478.

4.5.2.5 Dispersion Coefficients--

The model computes the longitudinal, lateral and vertical dispersion coefficients as the product of the seepage velocity and longitudinal (α_L), transverse (α_T) and vertical (α_V) dispersivities. A literature review indicated generalized theory to describe dispersivities, although a strong dependence on scale has been noted (Gelhar et al. 1985). In the absence of user-specified values, the model allows two alternatives.

Alternative 1, shown in Table 4-3(a), is based on the values presented in the Federal Register, Vol 51, No. 9, pp. 1652 (1986). These are:

$$\alpha_L = 0.1 x_r \quad (4-31)$$

$$\alpha_T = \frac{\alpha_L}{3.0} \quad (4-32)$$

where x_r = the distance to the receptor well [m]. Under this option, α_V is assumed to be uniformly distributed in the range of .0125 to .1 of the longitudinal dispersivity--i.e., in the range of 0.38 to 1.52 m.

Alternative 2 allows a probabilistic formulation for the longitudinal dispersivity as shown in Tables 4-3(a) and 4-3(b) [personal communication to Dr Zubair Saleem, Gelhar (1986)]. The longitudinal dispersivity is

Table 4-3(a). ALTERNATIVES FOR INCLUDING DISPERSIVITIES IN THE GROUNDWATER MODEL

Dispersivity	Alternative 1 Existing Values	Alternative 2 Gelhar's Recommendation
α_L (m)	15.24*	Probabilistic Formulation (see Table 4-3(b))
α_T (m)	5.07*	$\alpha_L/8$
α_V (m)	0.38-1.52	$\alpha_L/160$
α_L/α_T	3	8
α_L/α_V	10-40 (uniform distribution)	160

* Assumes $x_r = 152.4$ m (500 ft). Also see Equation 4-33.

Table 4-3(b). PROBABILISTIC REPRESENTATION OF LONGITUDINAL DISPERSIVITY FOR DISTANCE OF 152.4 m

Class	1	2	3
α_L (m)	0.1-1	1-10	10-100
Probability	0.1	0.6	0.3
Cumulative Probability	0.1	0.7	1.0

assumed to be uniform within each of the three intervals shown in Table 4-3(b). Note that these values of longitudinal dispersivity shown are based on a receptor well distance of about 152.4 m. For other distances, the following equation is used:

$$\alpha_L(x) = \alpha_L(x = 152)(x/152.4)^{0.5} \quad (4-33)$$

The transverse and vertical dispersivity are assumed to have the following values:

$$\alpha_T = \alpha_L/8 \quad (4-34)$$

$$\alpha_V = \alpha_L/160 \quad (4-35)$$

4.5.2.6 Recharge Rate into the Plume--

Recharge rate into the plume can be calculated by a variety of ways. One possibility is to use the HELP (Hydrologic Evaluation of Landfill Performance) model without any engineering controls (leachate collection system or a liner) to simulate the water balance for natural conditions. Results of such an analysis have been presented by E.C. Jordon Co. (1985 and 1987), and are included as default values in the model. This recharge is assumed to have no contamination and hence dilutes the groundwater plume.

4.5.3 Chemical-Specific Parameters

The model requires three chemical-specific parameters (see Table 4-1) that can be computed from the variables listed in Table 4-2. Note that chemical degradation within the saturated zone is limited to hydrolysis, and the by-products of hydrolysis are assumed to be non-hazardous.

4.5.3.1 Hydrolysis Rates--

The acid-catalysed, neutral and base-catalysed hydrolysis rates are all influenced by groundwater temperature. This effect is often quantified using the Arrhenius equation, which yields:

$$K_{a,n,b}^T = K_{a,n,b}^{T_r} \exp \left[E_a/R_g \left(\frac{1}{T_r + 273} - \frac{1}{T + 273} \right) \right] \quad (4-36)$$

where:

T = temperature of the groundwater [$^{\circ}\text{C}$]

T_r = reference temperature [$^{\circ}\text{C}$]

$K_{a,b}^{T_r}$ and $K_{a,b}^T$ = the second-order acid- and base-catalysis hydrolysis rate at temperature T_r and T respectively [l/mole-yr]

$K_n^{T_r}$ and K_n^T = the neutral hydrolysis rate at temperatures T_r and T respectively [l/yr]

R_g = universal gas constant [$1.987\text{E-}3 \text{ kcal/deg-mole}$]

E_a = Arrhenius activation energy [kcal/mole]

Note that, using the generic activation energy of 20 kcal/mole recommended by Wolfe (1985), the factor E_a/R_g has a value of about 10,000.

The acid-catalyzed, base-catalyzed and neutral hydrolysis rate constants can be combined (Mill et al. 1981) to yield the composite, first-order, dissolved-phase hydrolysis rate:

$$\lambda_1 = K_a^T [\text{H}^+] + K_n^T + K_b^T [\text{OH}^-] \quad (4-37)$$

where:

$[\text{H}^+]$ = the hydrogen ion concentration [mole/l]

$[\text{OH}^-]$ = the hydroxyl ion concentration [mole/l]

Note that $[H^+]$ and $[OH^-]$ can both be computed from the pH of the aquifer, i.e.,

$$[H^+] = 10^{-pH} \quad (4-38)$$

$$[OH^-] = 10^{-(14-pH)} \quad (4-39)$$

For the case of sorbed-phase hydrolysis, evidence suggests that base-neutralized hydrolysis can be neglected and that the acid-neutralized hydrolysis rate is enhanced by a factor of α . Thus, the effective sorbed-phase decay rate can be expressed as:

$$\lambda_2 = \alpha' K_a^T [H^+] + K_n^T \quad (4-40)$$

where α' = acid-catalysis hydrolysis rate enhancement factor for sorbed phase with a typical value of 10.0.

4.5.3.2 The Distribution Coefficient--

The relationship most suited for relating the chemical distribution coefficient, K_d , to soil or porous medium properties is discussed in detail by Karickhoff (1984). In the absence of user-specified values, hydrophobic binding is assumed to dominate the sorption process. For this case, the distribution coefficient can be related directly to soil organic carbon using:

$$K_d = K_{oc} f_{oc} \quad (4-41)$$

where:

- K_{oc} = normalized distribution coefficient for organic carbon
- f_{oc} = fractional organic carbon in the saturated zone

4.5.4 Receptor Well Location-Specific Parameters

Figure 4-3 is a schematic of the receptor well location relative to the waste facility. The location of the well is determined by specifying the radial distance to the well, angle between the plume centerline and the radial location of the well measured counterclockwise, and the depth of penetration of the well. Thus knowing these, the cartesian coordinates of the well location are computed as:

$$x_r = R \cos \psi \quad (4-42)$$

$$y_r = R \sin \psi \quad (4-43)$$

where:

R = the radial distance to the well [m]

ψ = the angle measured counterclockwise from the plume centerline
[degrees]

x_r, y_r = the cartesian coordinates of the well location [m]

In addition to the x and y coordinates, the z coordinate is specified as an input parameter and the well is assumed to have a single slot at that depth.

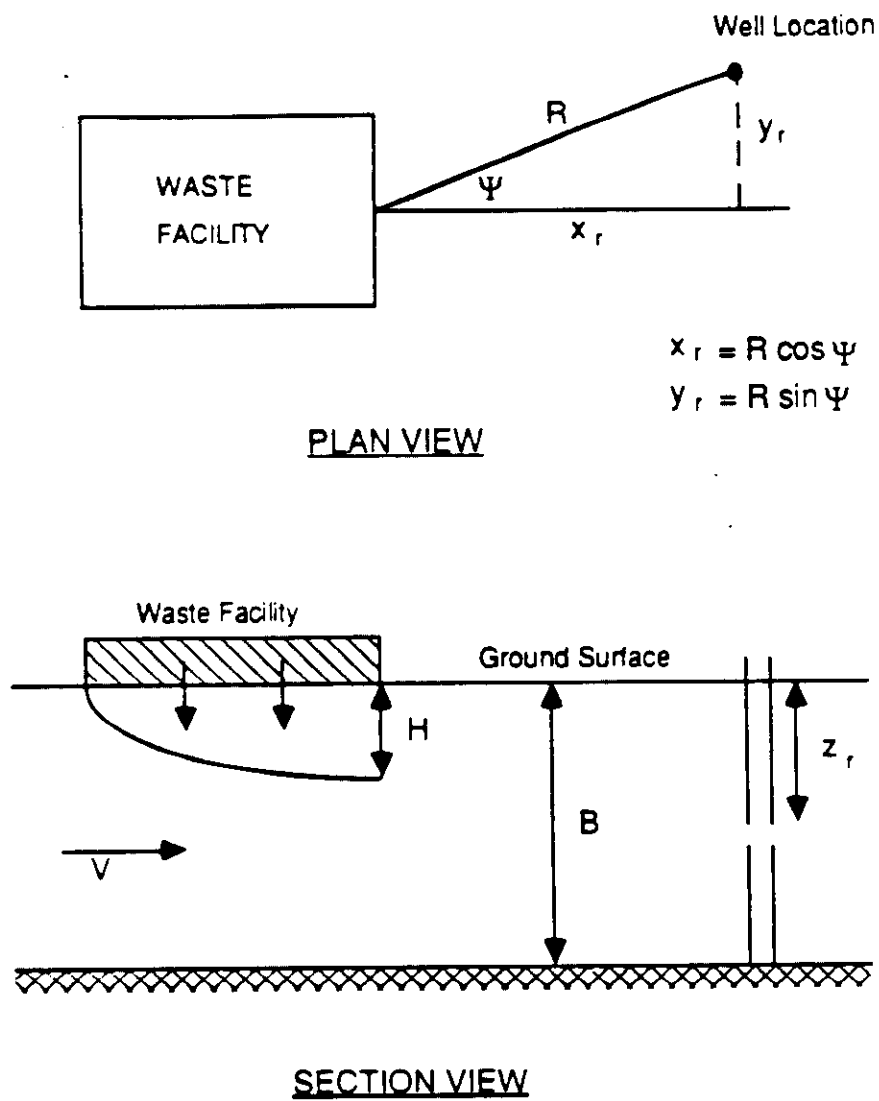


Figure 4-3. A Schematic of the Well Location

SECTION 5

UNCERTAINTY ANALYSIS

5.1 INTRODUCTION

As described in Section 1, EPACML simulates the movement of contaminants emanating from a waste disposal facility to a downgradient receptor well. The model includes algorithms that simulate the movement of the contaminant within the unsaturated zone and the saturated zone based on a number of user-specified parameters. These include chemical-specific, aquifer-specific, source-specific and receptor well location-specific parameters.

Typically the values of these parameters are not known exactly due to measurement errors and/or inherent spatial and temporal variability. Therefore, it is often more appropriate to express their value in terms of a probability distribution rather than a single deterministic value and to use an uncertainty propagation model to assess the effect of the variability on the model output.

This section presents the uncertainty propagation method implemented in the composite model. The method allows a quantitative estimate of the uncertainty in the downgradient receptor well location due to uncertainty in the model input parameters.

5.2 STATEMENT OF THE PROBLEM AND TECHNICAL APPROACH

The objective of the uncertainty analysis/propagation approach is to estimate the uncertainty in the receptor well concentration given the

uncertainty in the input parameters. Alternatively, the objective is to estimate the cumulative probability distribution of the downgradient well concentration given the probability distribution of the input parameters. Thus if C_w represents the downgradient well concentration and \underline{X} represents the vector of all model inputs:

$$C_w = g(\underline{X}) \quad (5-1)$$

where g represents the semi-analytical, composite model. Note that some or all of the components of \underline{X} may vary in an uncertain way, i.e., they are random variables defined by cumulative probability distribution functions. Thus the goal here is to calculate the cumulative distribution function $F_{C_w}(C'_w)$ given a probabilistic characterization of \underline{X} . Note that $F_{C_w}(C'_w)$ is defined as:

$$F_{C_w}(C'_w) = \text{Probability } (C_w \leq C'_w) \quad (5-2)$$

where C'_w is a given downgradient well concentration.

To our knowledge, five main methods have been proposed to evaluate $F_{C_w}(C'_w)$. These include:

1. First-Order and First-Order-Second-Moment Analysis (FO, FOSM);
2. Monte Carlo Simulation (MC);
3. Discretization of Probability Distributions (DPD);
4. Response Surface Analysis (RS); and
5. Rackwitz-Fiessler Method and its variants (RF).

These methods were evaluated by U.S. EPA in order to select the most appropriate method for uncertainty analysis using the composite model. The selection criteria included:

1. Computation efficiency, measured by the number of response calculations required to achieve a given level of precision in estimation of the output statistic (in this case, the 85th percentile of the output distribution).
2. Accuracy in evaluation of the output statistic--e.g., a specified percentile value.
3. Generality of application, so that a number of modules and input conditions, and all sources of uncertainty, can be accommodated by the same uncertainty-propagation method.
4. Simplicity of usage, measured by the number of parameters that must be specified by the user for each application.
5. Completeness of the information produced, which may include only the mean and variance of the output distribution or may be the whole distribution, and which may or may not contain information useful for uncertainty decomposition.
6. Flexibility with respect to input distributions, so that the method would be able to accommodate a number of different input distributions.

Using the above criteria, a qualitative comparison of the various uncertainty-propagation methods is included in Table 5-1.

With the above criteria in mind and knowledge of the composite model, the Monte Carlo Analysis method was selected. This approach is simple,

Table 5-1. QUALITATIVE COMPARISON OF UNCERTAINTY-PROPAGATION METHODS

Criterion	UNCERTAINTY PROPAGATION METHOD				
	FO, FOSM	MC	DPD	RS	RF
Computational Efficiency	***	**		**	*
Accuracy	*	*	*	**	**
Generality	**	***	*	*	*
Simplicity	***	***	***	**	*
Information Produced	**	*	**	**	***
Variation of $F_{\underline{X}}$	**	**	**	***	*

no star - criteria not satisfied

* - criteria partially satisfied

** - criteria satisfied in general

*** - criteria satisfied

unbiased and completely general. Also, the method is especially attractive when there are many input variables that are randomly distributed, because the efficiency does not depend on the dimensionality of the input vector. Further, since the composite model is analytical, it would not be very expensive to run a large number of independent executions of the model to achieve satisfactory confidence limits on the downgradient well concentration. Details of this method are discussed below.

5.3 THE MONTE CARLO ANALYSIS TECHNIQUE

Figure 5-1 illustrates the Monte Carlo method used in this analysis. Given a set of deterministic values for each of the input parameters, X_1, X_2, \dots, X_n , the composite model computes the downgradient receptor well concentration C_w , i.e.:

$$C_w = g(X_1, X_2, X_3, \dots, X_n) \quad (5-3)$$

Application of the Monte Carlo simulation procedure requires that at least one of the input variables, X_1, \dots, X_n , be uncertain and the uncertainty represented by a cumulative probability distribution. The method involves the repeated generation of pseudo-random values of the uncertain input variable(s) (drawn from the specified distribution and within the range of any imposed bounds) and the application of the model using these values to generate a series of model responses, i.e., values of C_w . These responses are then statistically analyzed to yield the cumulative probability distribution of the model response. Thus, the various steps involved in the application of the Monte Carlo simulation technique involve:

- i) Selection of representative cumulative probability distribution functions for the relevant input variables

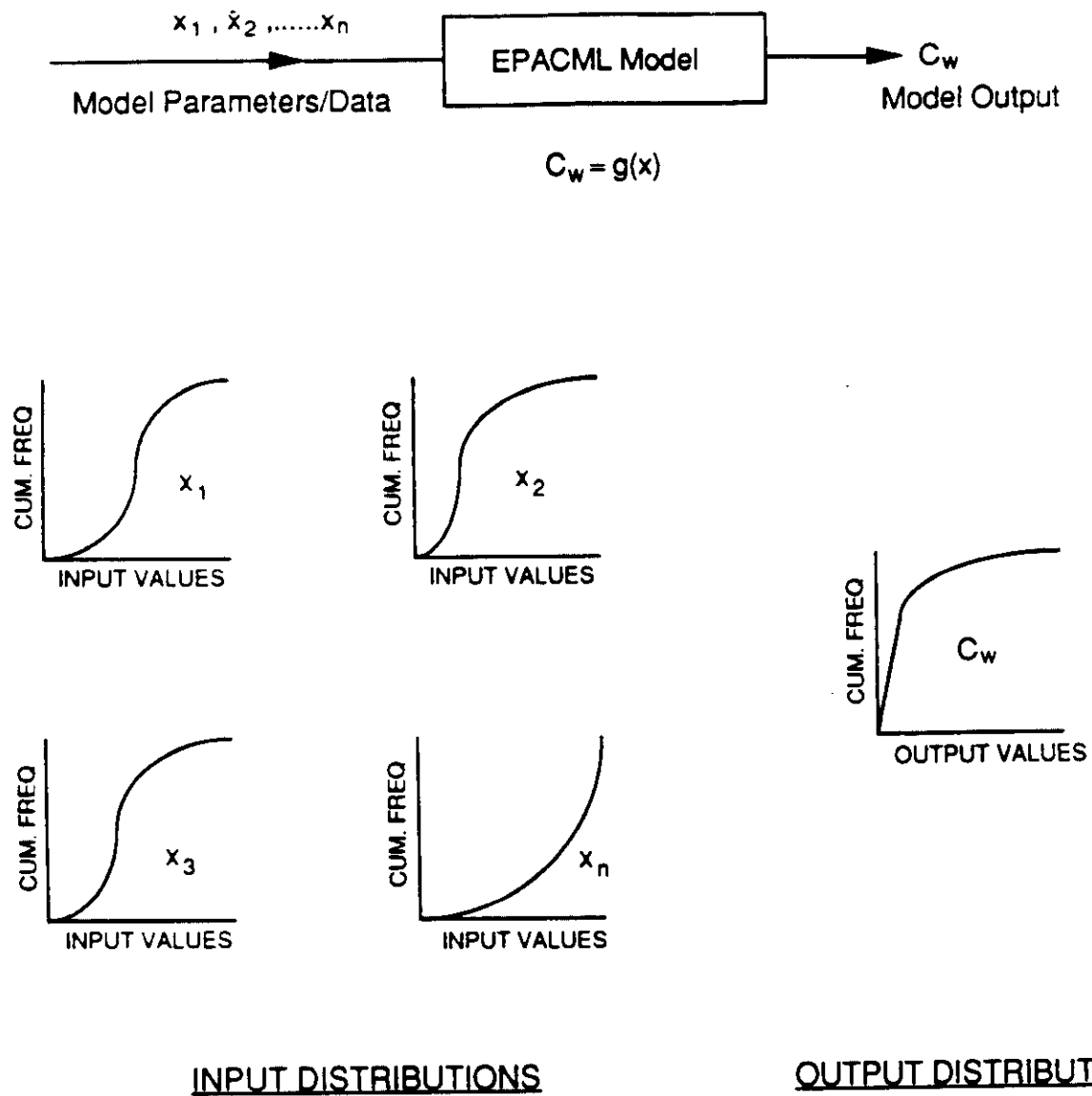


Figure 5-1. A Schematic Description of the Monte Carlo Method of Uncertainty Analysis

- ii) Generation of a pseudo-random number from the distributions selected in (i). These values represent a possible set of values for the input variables
- iii) Application of the model to compute the derived inputs and output(s)
- iv) Repeated application of steps (ii) and (iii)
- v) Presentation of the series of output (random) values generated in step (iii) as a cumulative probability distribution function (CDF)
- vi) Further analysis and application of the cumulative probability distribution as a tool for decision making

5.4 UNCERTAINTY IN THE INPUT VARIABLES

The variables required by the composite model can be broadly classified into two different sets that exhibit different uncertainty characteristics. These are:

- i) Variables that describe the chemical, biochemical, and toxicological properties of the hazardous constituent. Examples of these variables include the octanol-water partition coefficient; acid-, neutral, and base-catalyzed hydrolysis rate; soil adsorption coefficient; etc.
- ii) Variables that describe the environmental properties of the various media and impact the fate and transport of the pollutant within each medium. Examples of these variables include the groundwater velocity, soil porosity, organic carbon content, dispersivity values, etc.

Uncertainty in the first set of variables primarily arises due to laboratory measurement errors or theoretical analysis used to estimate the numerical values. In addition to experimental precision and accuracy, errors may arise due to extrapolations from controlled (laboratory) measurement conditions to uncontrolled environmental (field) conditions. Further, for some variables, semi-empirical methods are used to estimate the values. In this case, errors in using the empirical relationships also contribute to variability in the model outputs.

Uncertainty in the second set of variables, identified above, may include both measurement and extrapolation errors. However, the dominant source of uncertainty in these is the inherent natural (spatial and temporal) variability. This variability can be interpreted as site-specific or within-site variation in the event that the model is used to analyze exposure due to a specific land-disposal unit. Alternatively it can represent a larger-scale (regional/national) uncertainty if the model is used to conduct exposure analysis for a specific chemical or specific disposal technology on a generic, nationwide or regional basis. Note that the distributional properties of the variables may change significantly depending upon the nature of the application.

Whatever the source of uncertainty, the uncertainty preprocessor developed for the composite model requires that the uncertainty be quantified by the user. This implies that for each input parameter deemed to be uncertain, the user select a distribution and specify the parameters that describe the distribution.

The current version of the preprocessor allows the user to select one of the following distributions:

- i) Normal
- ii) Lognormal
- iii) Uniform

- iv) Log uniform
- v) Exponential
- vi) Empirical
- vii) Johnson SB

The first two distributions require the user to specify the mean and the variance. The third and the fourth require minimum and maximum values. The fifth distribution requires only one parameter: the mean of the distribution. For the empirical distribution, the user is required to input the coordinates of the cumulative probability distribution function (minimum 2 pairs, maximum 20 pairs), which is subsequently treated as a piece-wise linear curve. Finally, the Johnson SB distribution requires four parameters: mean, variance, the lower and upper bounds.

Of the above seven distributions, the characteristics of the first six are readily available in literature (Benjamin and Cornell 1970). However details of the Johnson SB distribution may not be as readily available. Consequently a brief description of this distribution is presented below.

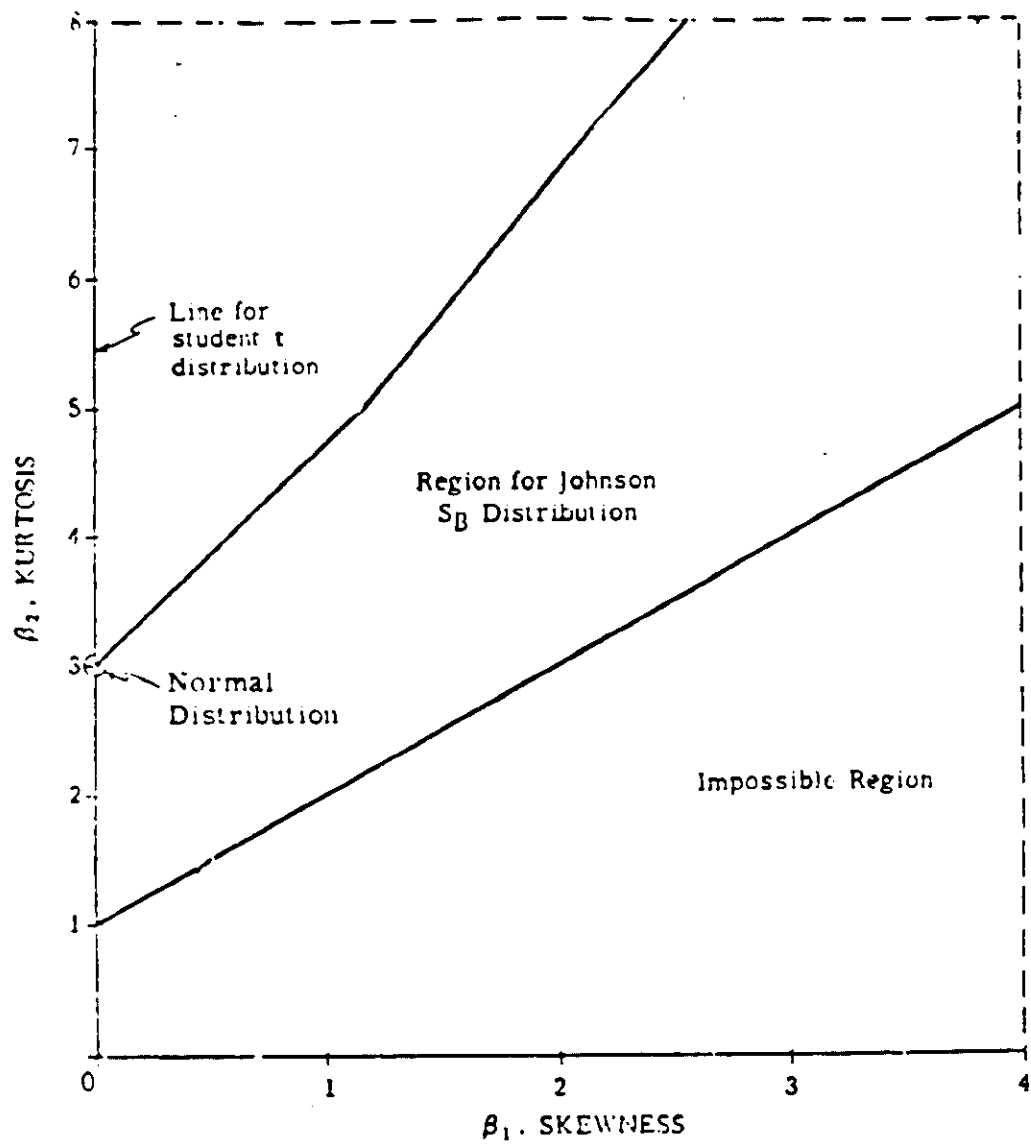
This distribution represents a transformation applied to the random variable such that the transformed variable is normally distributed. The specific transformation is:

$$SB: Y = \ln\left(\frac{X-A}{B-X}\right) \quad (5-5)$$

where:

- \ln = natural logarithm transformation
- X = untransformed variable with limits of variation from A to B
- Y = the transformed variable with a normal distribution

Selection of the Johnson SB distribution for a sample data set is accomplished by plotting the skewness and kurtosis of the sample data as shown in Figure 5-2. The location of the sample point indicates the



Source: McGrath et al. 1973

Figure 5-2. Selecting a Johnson Distribution from Skewness and Kurtosis

distribution for the sample data. For additional details of the Johnson distribution, the reader is referred to McGrath and Irving (1973) and Johnson and Kotz (1970).

5.5 THE RANDOM NUMBER GENERATOR

Having selected the distribution for the various input parameters, the next step is the generation of random values of these parameters. This requires the use of pseudo-random number generating algorithms. There exist numerous non-proprietary subroutines that can be used to generate random numbers. A number of these are comparable in terms of their computational efficiency, accuracy and precision. The specific routines included in the composite code are those described by McGrath and Irving (1973). The performance of these algorithms has been checked to ensure that they accurately reproduce the parameters of the distributions that are being sampled as described below.

In order to test the algorithms, two sets of runs were made. For Run 1, 500 random numbers were generated; for Run 2, 1000 random numbers were generated. For the five distributions tested, the input parameters and the results are shown in Tables 5-2(a) and (b). In each case, the output statistics for the randomly generated variables closely match the input values. Additional testing using the bootstrap method has been performed by the Agency to estimate the number of runs.

For Run 2, the randomly generated variables were arranged in ascending order and the cumulative probability distributions of the generated variable plotted and compared with the theoretically exact/expected distributions. These are shown in Figures 5-3 to 5-7. Visual inspection of these figures further testify to the accuracy of these algorithms.

Note that more rigorous statistical tests could be used to further test the accuracy of the algorithms. However, the above simplified analysis has provided sufficient proof of the accuracy of the results and indicated that these algorithms satisfactorily reproduce the input statistics and distributions of the variables.

Table 5-2(a). RESULTS OF RANDOM NUMBER GENERATOR TEST FOR 500 VALUES

	Input Statistics		Observed Output Statistics			
	mean	std. dev.	mean	std. dev.	max	min
Normal	10.00	1.00	10.00	1.05	13.40	6.90
LogNormal	10.00	1.00	9.97	0.98	13.20	7.60
Exponential	10.00	10.00	9.80	9.67	53.70	0.00
Empirical*	18.855	-	18.54	25.54	99.20	0.10
Uniform	10**	25***	17.4	--	24.9	10.1

*Cumulative Probability 0.0 0.1 0.7 1.0
 Values 0.1 1.0 10.0 100.0
 Expected Mean 18.855

**Minimum Value

***Maximum Value

Table 5-2(b). RESULTS OF RANDOM NUMBER GENERATOR TEST FOR 1000 VALUES

	Input Statistics		Observed Output Statistics			
	mean	std. dev.	mean	std. dev.	max	min
Normal	10.00	1.00	9.99	1.00	13.60	7.25
LogNormal	10.00	1.00	9.97	0.99	14.50	7.26
Exponential	10.00	10.00	9.77	10.04	86.20	0.15
Empirical*	18.855	-	21.57	28.16	99.80	0.11
Uniform	10**	25***	17.41	4.26	25.00	10.00

*Cumulative Probability 0.0 0.1 0.7 1.0
 Values 0.1 1.0 10.0 100.0
 Expected Mean 18.855

**Minimum Value

***Maximum Value

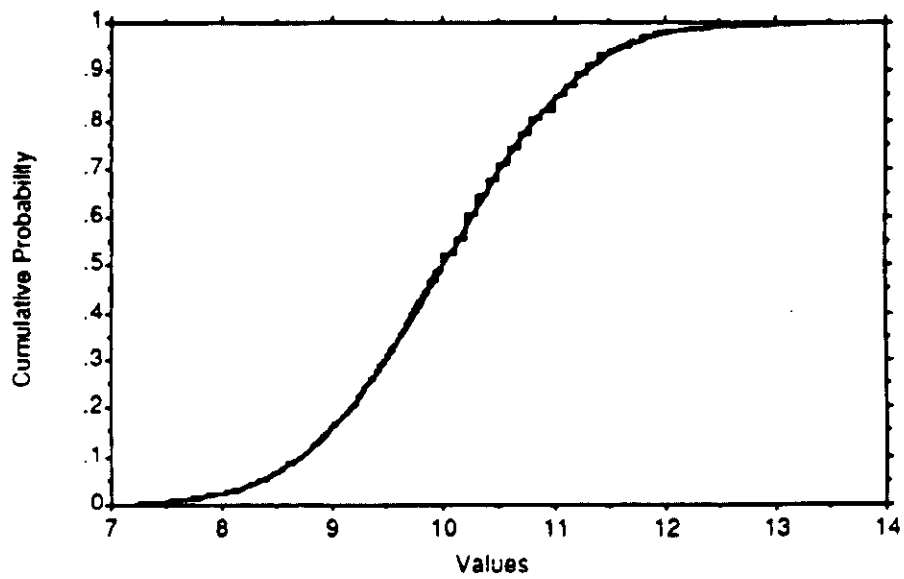


Figure 5-3. Comparison of the Exact and the Generated Cumulative Frequency Distribution for a Normally Distributed Variable

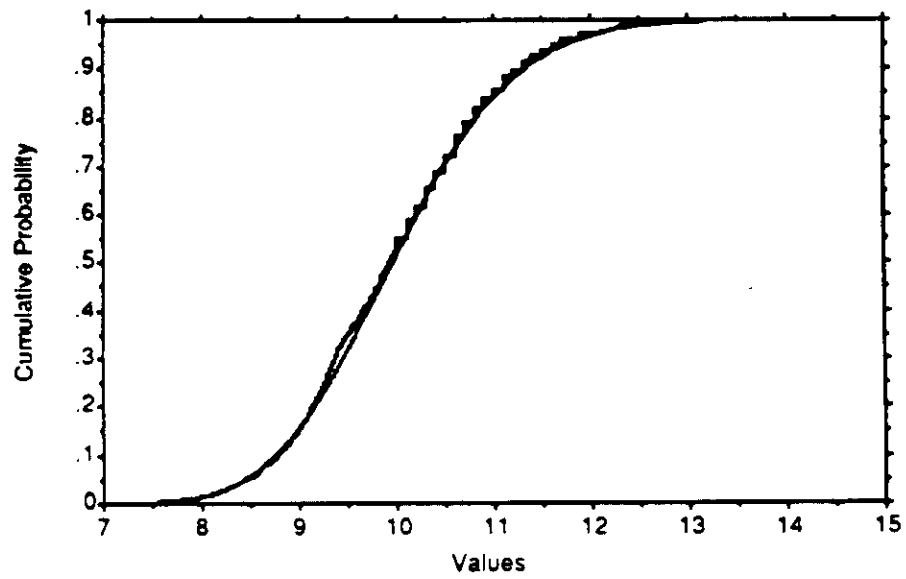


Figure 5-4. Comparison of the Exact and the Generated Cumulative Frequency Distribution for a Log Normally Distributed Variable

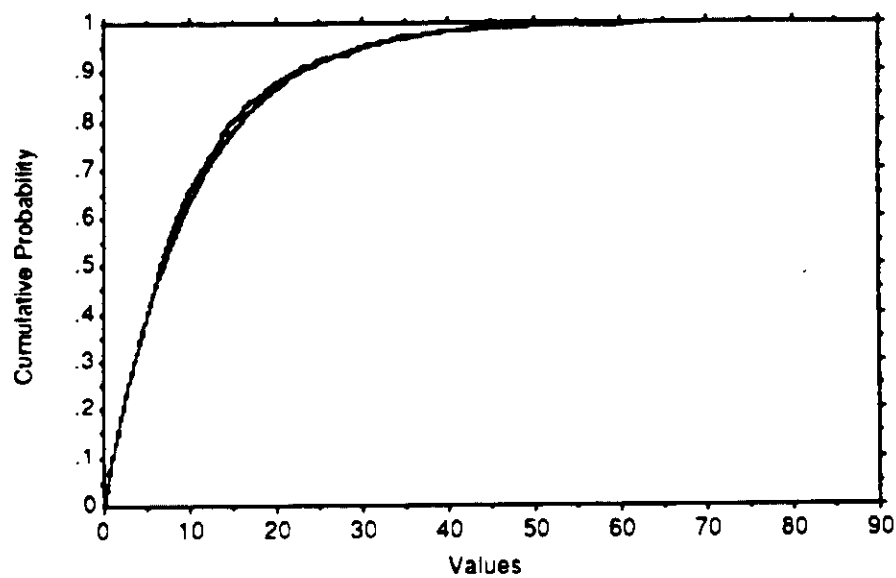


Figure 5-5. Comparison of the Exact and the Generated Cumulative Frequency Distribution for an Exponentially Distributed Variable

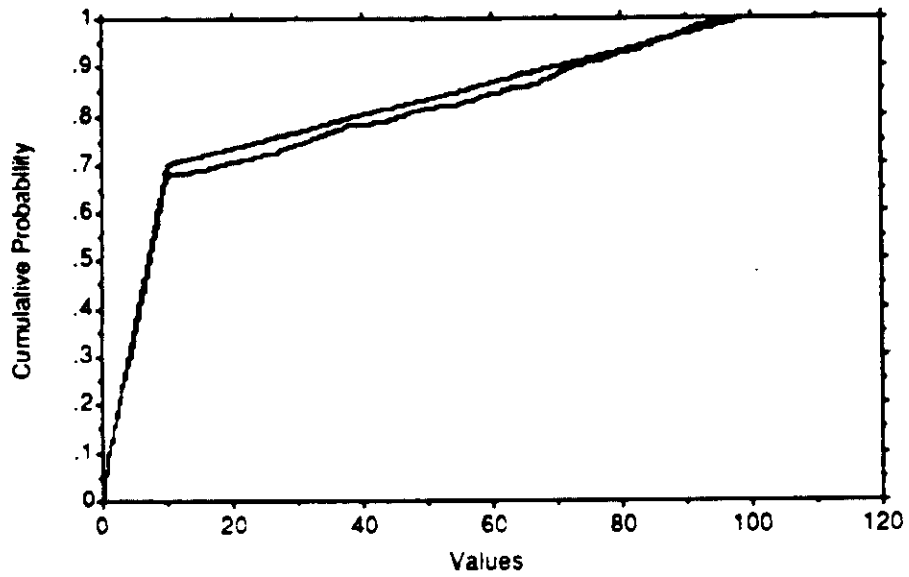


Figure 5-6. Comparison of the Exact and the Generated Cumulative Frequency Distribution for an Empirically Distributed Variable

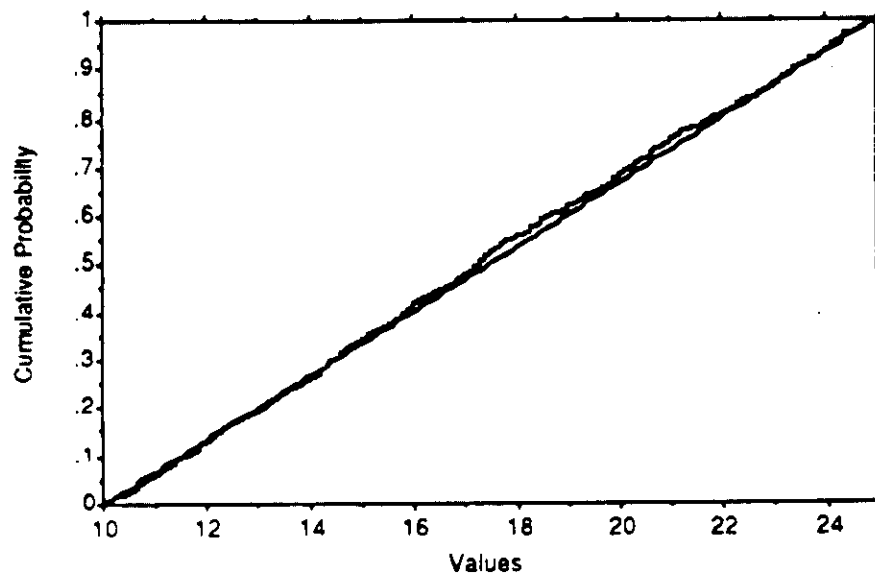


Figure 5-7. Comparison of the Exact and the Generated Cumulative Frequency Distribution for a Uniformly Distributed Variable

5.6 ANALYSIS OF THE MODEL OUTPUT

Using the randomly generated parameter values, the model is used to estimate values of concentrations at various points located downgradient from the waste facility. Thus, if C_w represents the normalized (with the leachate concentration at the waste facility) receptor well concentration calculated by the model assuming that the leachate concentration at the waste disposal facility is unity, and C_T is the (health-based maximum allowable) threshold concentration for the chemical at the receptor well, the maximum allowable leachate concentration at the waste facility can be back-calculated using:

$$C_L = \frac{C_T}{C_w} \quad (5-6)$$

Note that the maximum allowable leachate concentration defined by Equation 5-6 is the leachate concentration for which the downgradient receptor well concentration does not exceed the threshold concentration. Alternatively,

$$\frac{1}{C_w} = \frac{C_L}{C_T} \quad (5-7)$$

Equation 5-7 states that the reciprocal of the computed normalized concentration represents the maximum allowable ratio of leachate concentration to the threshold concentration. Thus, for example, if the simulated normalized concentration $C_w = 0.05$, Equation 5-7 implies that the maximum allowable leachate concentration from the landfill could be 20 times the threshold value for the chemical. Note that both C_w and C_T are chemical specific.

The above back-calculation procedure and the Monte Carlo analysis allows the maximum leachate concentration to be couched in a probabilistic framework. Thus for each chemical, the maximum allowable leachate concentration is chosen by considering the percentage of feasible nationwide sites, p , for which the resulting downgradient concentrations are in compliance with established standards. This is further explained below.

Application of the above Monte Carlo method results in an array of values for the model output (normalized concentration), each representing a feasible waste disposal facility-environmental scenario. These values are statistically analyzed to derive the cumulative probability distribution function as shown in Figure 5-8. The cumulative probability distribution, $F_{C_w}(C_w)$, together with the allowable threshold value, C_T , and the back calculation procedure (Equations 5-6 and 5-7), provide the information necessary to calculate the maximum allowable leachate concentration. In particular the value of leachate concentration C_l that leads to p% of the sites in compliance--i.e., the receptor well concentration is less than or equal to the threshold concentration--is:

$$C_l = \frac{C_T}{C_p} \quad (5-8)$$

where C_p is the p percentile concentration obtained from the cumulative distribution function of the downgradient well concentration. Note that for the current regulation, the maximum allowable leachate concentration C_l is chosen such that at least $p = 85\%$ of the sites are in compliance.

5.7 IMPLEMENTATION OF THE MONTE CARLO SIMULATION PROCEDURE

The immediate objective of the Agency is to run the composite model in the Monte Carlo mode and develop the chemical-specific cumulative frequency distribution of the normalized downgradient well concentration that is representative of nationwide uncertainty in the model parameters. For policy development/analysis purposes, the Agency plans to select a specific (e.g., 85th) percentile of the normalized concentration and compute the maximum leachate concentration using Equation 5-8. The percentile is selected from a cumulative distribution of the normalized concentrations that are representative of nationwide variation in the model input parameters. This nationwide variation is represented by dividing the

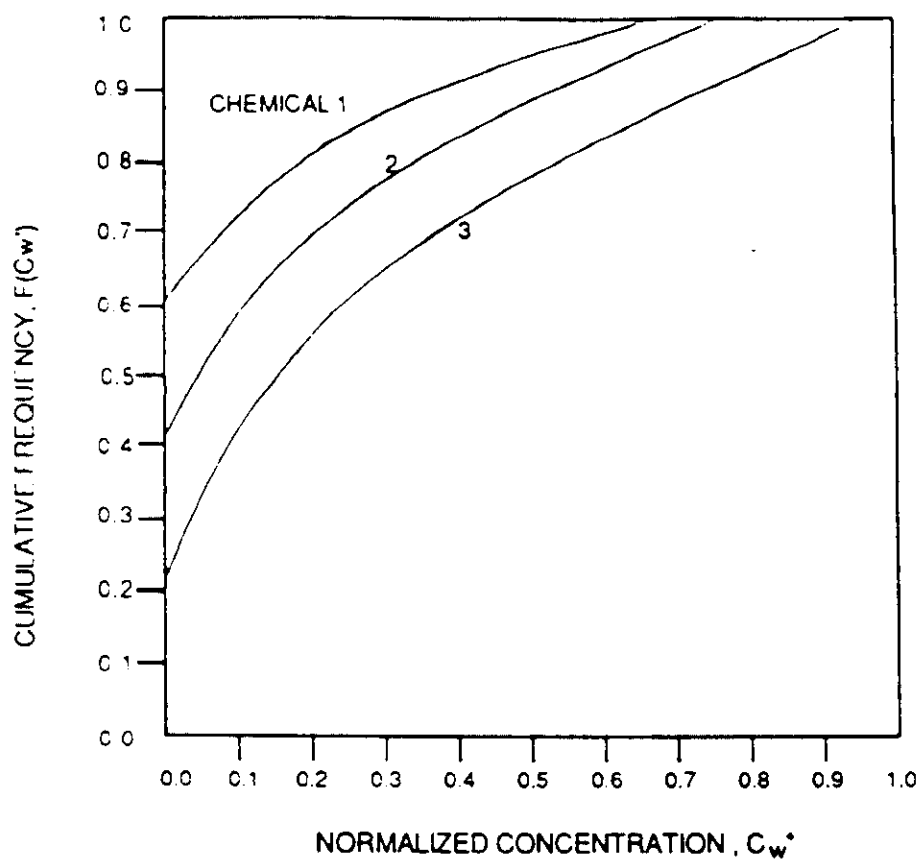


Figure 5-8. Typical Results Obtained Using EPACML in the Monte Carlo Mode

* Normalized with respect to source concentration

nation into nine hydrogeologic settings--each with a different combination of unsaturated soil type and infiltration rate. Other inputs--e.g., aquifer-, chemical-, and receptor well-specific parameters--are considered the same for each of these nine settings.

For each chemical, nine Monte Carlo simulations using the composite model each representative of a hydrogeologic setting and described above are conducted. Data used for the saturated zone transport computations are presented in Section 4. The model results, normalized concentrations at the downgradient well, were used to derive the cumulative probability distribution function for each soil type. These individual distributions were then combined together using weighting factors for the hydrogeologic settings (relative nationwide occurrence of each hydrogeologic setting) to estimate the composite distribution based on the total probability theorem. Thus, the composite probability of a concentration C'_w is given by:

$$F_C(C_w = C'_w) = \sum_{I=1}^9 F(C_w = C'_w | I) P_I \quad (5-9)$$

where

C'_w = a specified concentration value

$F_C(C_w = C'_w)$ = probability that the composite (nationwide) normalized concentration is less than or equal to C'_w

$F(C_w = C'_w | I)$ = probability that the concentration is less than or equal to C'_w for hydrogeologic setting I

P_I = probability of occurrence of hydrogeologic setting I

Having thus derived $F_C(C_w)$ --the composite nationwide cumulative probability distribution--the maximum leachate concentration for a specified percentile can be obtained and interpreted for regulatory purposes as described in Section 5.2 and Equation 5-8.

The composite model code, EPACML, includes an uncertainty post-processor that can be used to derive the cumulative distribution function,

and specified percentiles of that function. Further, printer plots of the cumulative frequency distribution of the concentration at the receptor well location can also be obtained.

SECTION 6

DEFAULT INPUT DATA FOR EPACML

6.1 INTRODUCTION

The EPACML model requires five groups of data; chemical-specific data, source-specific data, unsaturated zone flow data, unsaturated zone transport data, and aquifer-specific data. A brief discussion of each data group and the values used for the base case simulation for each of the variables within the group is given below.

6.2 CHEMICAL-SPECIFIC DATA GROUP

The chemical-specific data group contains the parameters required to calculate the overall decay rate and the retardation coefficient of the chemical being simulated for the unsaturated and the saturated zones. Table 6-1 shows the parameters in the chemical-specific data group for a conservative chemical. Each of the parameters is discussed below.

6.2.1 Decay Coefficient

The overall decay coefficient for a chemical is the weighted average of the dissolved and sorbed phase decay coefficients as discussed in Section 4.2. The dissolved and the solid phase decay coefficients are derived from values of chemical specific hydrolysis rate constants, and the pH, temperature, bulk density and porosity of the aquifer. (The latter are included in the aquifer-specific data group and discussed in Section 6.6).

Table 6-1. PARAMETERS INCLUDED IN THE CHEMICAL-SPECIFIC DATA GROUP OF EPACML MODEL

CHEMICAL SPECIFIC VARIABLES						
VARIABLE NAME	UNITS	DISTRIBUTION	PARAMETERS		LIMITS	
			MEAN	STD DEV	MIN	MAX
Solid phase decay coefficient	1/yr	DERIVED	.000E+00	.000E+00	.000E+00	.352E+05
Dissolved phase decay coefficient	1/yr	DERIVED	.000E+00	.000E+00	.000E+00	.221E+09
Overall chemical decay coefficient	1/yr	DERIVED	.000E+00	.000E+00	.000E+00	.358E+05
* Acid catalyzed hydrolysis rate	l/M-yr	CONSTANT	.000E+00	.000E+00	.000E+00	.000E+00
* Neutral rate constant	1/yr	CONSTANT	.000E+00	.000E+00	.000E+00	.000E+00
* Base catalyzed hydrolysis rate	l/M-yr	CONSTANT	.000E+00	.000E+00	.000E+00	.000E+00
Reference temperature	C	CONSTANT	25.0	.000E+00	.000E+00	40.0
* Normalized distribution coefficient	ml/g	CONSTANT	.000E+00	.000E+00	.000E+00	.000E+00
Distribution coefficient	--	DERIVED	.219	.000E+00	.000E+00	.166E+05
Biodegradation coefficient (sat. zone)	1/yr	CONSTANT	.000E+00	.000E+00	.000E+00	100.

78

* These values vary depending on the chemical being simulated

6.2.2 Chemical Specific Hydrolysis Rate Constants

Table 6-2 presents the values of the hydrolysis rates for a conservative chemical, chlordane and chloroform, at a reference temperature of 25°C.

6.2.3 Distribution Coefficient

The distribution coefficient is calculated as the product of the normalized distribution coefficient and the fractional organic carbon content in the aquifer. The normalized distribution coefficients used in the simulations are given in Table 6-2. The value of organic carbon content of the aquifer is discussed with the aquifer-specific data in Section 6.6.

6.2.4 Biodegradation Coefficient

For these simulations, biodegradation as a mechanism was neglected, i.e., the biodegradation coefficient was set to zero.

6.3 SOURCE-SPECIFIC DATA GROUP

The source-specific data group describes the geometry, leachate rate and contaminant source characteristics for the landfill. Table 6-3 shows the parameters included in this group. A description of each parameter is given below.

6.3.1 Infiltration Rate

Three different empirical cumulative probability distributions for infiltration rate were used, each corresponding to a different cover soil type for the landfill. These distributions were derived using the HELP model (E.C. Jordan 1985 and 1987). Table 6-4 and Figure 6-1 present these distribution.

Table 6-2. CHEMICAL SPECIFIC PROPERTIES USED IN SIMULATIONS

	Acid Catalyzed Hydrolysis ($\mu\text{M-yr}$)	Base Catalyzed Hydrolysis ($\mu\text{M-yr}$)	Neutral Rate Constant (1/yr)	Normalized Distribution Coefficient (ml/g)
Conservative Chemical	0.0	0.0	0.0	0.0
Chloroform	0.0	.21E+04	.23E-04	39.8
Chlordane	0.0	37.7	0.0	.331E+06

Table 6-3. PARAMETERS INCLUDED IN THE SOURCE-SPECIFIC DATA GROUP OF EPACML MODEL

SOURCE SPECIFIC VARIABLES										
VARIABLE NAME	UNITS	DISTRIBUTION	PARAMETERS		LIMITS		MIN	MAX		
			MEAN	STD DEV						
* Infiltration rate	m/yr	EMPIRICAL	.510E-01	.500E-02			.100E-04	1.00		
* Area of waste disposal unit	m ²	NORM. TRANSF.	4.21	2.16			.884	12.3		
Duration of pulse	yr	CONSTANT	.100E+31	3.00			.100	.100E+31		
Spread of contaminant source	m	DERIVED	50.0	.000E+00			.100E-02	.600E+05		
* Recharge rate	m/yr	EMPIRICAL	.510E-01	.500E-02			.100E-04	1.00		
Source decay constant	1/yr	CONSTANT	.000E+00	.000E+00			.000E+00	10.0		
Initial concentration at landfill	mg/l	CONSTANT	1.00	.100E-01			.000E+00	10.0		
Length scale of facility	m	DERIVED	100.	1.00			1.00	.100E+06		
Width scale of facility	m	DERIVED	100.	1.00			1.00	.100E+06		
EMPIRICAL CUMULATIVE DISTRIBUTIONS										
Infiltration rate for silt loam soil cover										
PROBABILITIES	.000	.260	.310	.498	.548	.624	.674	.726	.746	.771
.801	.851	.865	.871	.901	.905	.914	.964	.980	1.000	
VALUES	.000E+00	.100E-02	.300E-02	.500E-02	.100E-01	.530E-01	.890E-01	.102	.109	.124
.127	.147	.175	.185	.216	.231	.251	.267	.274	.787	
Recharge rate for sandy loam soil type										
PROBABILITIES	.000	.030	.080	.130	.260	.290	.400	.478	.498	.540
.590	.650	.700	.755	.803	.833	.880	.930	.980	1.000	
VALUES	.000E+00	.180E-01	.380E-01	.660E-01	.710E-01	.760E-01	.104	.142	.147	.211
.229	.295	.310	.366	.401	.475	.495	.638	.729	1.06	

* Infiltration and recharge vary depending on cover soil type and unsaturated zone soil type respectively (Sections 6.3.1 and 6.3.5)
Area varies for landfill or surface impoundment scenarios (Section 6.3.2)

Table 6-4. EMPIRICAL DISTRIBUTIONS USED TO REPRESENT INFILTRATION
RATE (m/yr) THROUGH SUBTITLE D LANDFILL

COVER SOIL TYPE					
Silt Loam		Sandy Loam		Silty Clay Loam	
Cumulative Probability (%)	Rate (m/yr)	Cumulative Probability (%)	Rate (m/yr)	Cumulative Probability (%)	Rate (m/yr)
0.0	0.000	0.0	0.000	0.0	2.54E-5
26.0	0.001	3.0	0.018	57.0	0.00762
31.0	0.003	8.0	0.038	57.0	0.0330
49.8	0.005	13.0	0.066	64.0	0.0508
54.8	0.010	26.0	0.071	73.0	0.0787
62.4	0.053	29.0	0.076	73.0	0.0991
67.4	0.089	40.0	0.104	89.0	0.129
72.6	0.102	47.8	0.142	93.0	0.152
74.6	0.109	49.8	0.147	96.0	0.191
77.1	0.124	54.0	0.211	99.0	0.211
80.1	0.127	59.0	0.229	99.0	0.246
85.1	0.147	65.0	0.295	100.0	0.688
86.5	0.175	70.0	0.310		
87.1	0.185	75.5	0.366		
90.1	0.216	80.3	0.401		
90.5	0.231	83.3	0.475		
91.4	0.251	88.0	0.495		
96.4	0.267	93.0	0.638		
98.0	0.274	98.0	0.729		
100.0	0.787	100.0	1.064		

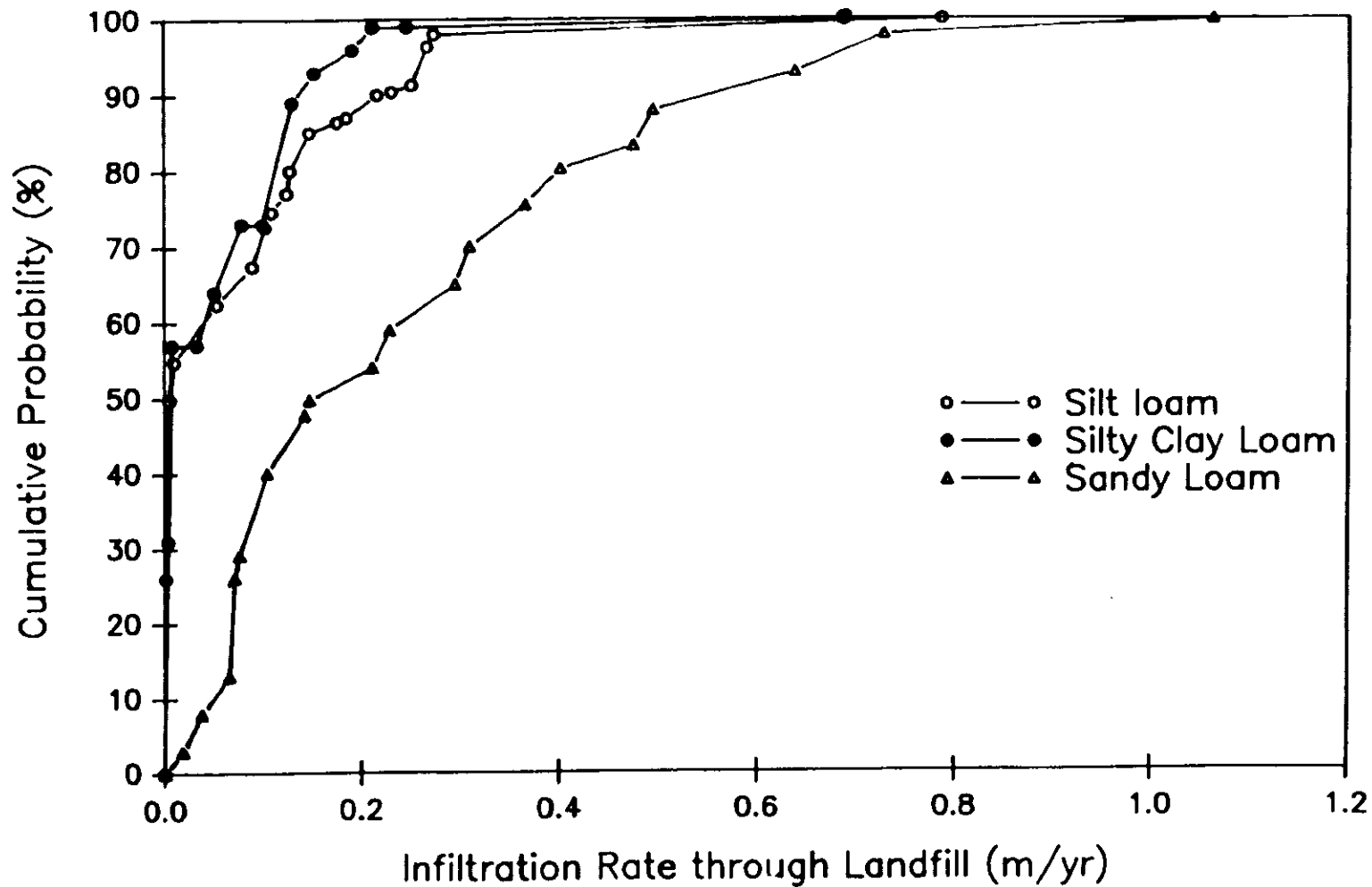


Figure 6-1. Empirical Distribution Used to Represent the Infiltration Rate through a Subtitle D Landfill

6.3.2 Area of Facility

A transformed normal distribution was used to represent the area of the landfill (U.S. EPA 1988). For this case, a normally distributed number (AT) (with mean = 4.21, standard deviation of 6.16 and minimum and maximum values of -.884 and 12.3, respectively) is first generated and then transformed to the actual area using:

$$AW = [(AT * 0.08 + 1)^{(1/0.08)} + 0.6] * 4047 \quad (6.1)$$

where

AW = the area of the facility [m²]
AT = the normally distributed variable
4047 = converts acres to m²

6.3.3 Duration of Pulse

All simulations were performed for steady-state, hence the duration of the pulse was set to a very large number.

6.3.4 Spread of the Contaminant Source

The spread of the contaminant source in the saturated zone was calculated as one-sixth of the facility width.

6.3.5 Recharge Rate

The ambient recharge rate was estimated using the same distributions as the infiltration rates (see Table 6-4). Three different distributions were used depending upon the unsaturated zone soil underlying the facility (also see Section 6.5).

6.3.6 Source Decay Constant

For the steady-state simulations presented in this report, the source decay rate was set to zero.

6.3.7 Initial Concentration at Source

A continuous source with a constant concentration of unity was assumed. Hence, the model output is the normalized concentration of the chemical at the downgradient well.

6.3.8 Length Scale of the Facility

The length scale of the facility was calculated as the square root of the area.

6.3.9 Width Scale of the Facility

The width scale of the facility was calculated as the square root of the area.

6.4 UNSATURATED ZONE FLOW DATA GROUP

The unsaturated zone flow data shown in Table 6-5, consists of three subgroups that include the unsaturated zone control parameter group, the material variables and the functional variables. Data in each of these groups is discussed below.

6.4.1 Control Parameter Subgroup

Table 6-5 lists the values assigned to the control parameters. Since the depth of the unsaturated zone is randomly generated (see Section 6.4.2) the spatial discretization required for the numerical solution of the unsaturated zone flow equation, was performed automatically by the model

Table 6-5. PARAMETERS INCLUDED IN THE UNSATURATED ZONE FLOW DATA GROUP OF EPACML MODEL

UNSATURATED ZONE FLOW MODEL PARAMETERS

(input parameter description and value)

NP	- Total number of nodal points	7
NMAT	- Number of different porous materials	1
KPROP	- Van Genuchten or Brooks and Corey	1
IMSHGN	- Spatial discretization option	1

OPTIONS CHOSEN

Van Genuchten functional coefficients

DATA FOR MATERIAL 1

VADOSE ZONE MATERIAL VARIABLES

VARIABLE NAME	UNITS	DISTRIBUTION	PARAMETERS		LIMITS	
			MEAN	STD DEV	MIN	MAX
* Saturated hydraulic conductivity	m/yr	SB	2.30	24.7	.000E+00	30.0
* Vadose zone porosity	--	CONSTANT	.410	.000E+00	.000E+00	.500
* Air entry pressure head	m	CONSTANT	.000E+00	.000E+00	.000E+00	1.00
Depth of the unsaturated zone	m	EMPIRICAL	6.10	1.00	.610	366.

EMPIRICAL CUMULATIVE DISTRIBUTIONS

Depth of the unsaturated zone

PROBABILITIES	.000	.050	.100	.200	.250	.300	.350	.400	.450	.500
.600	.650	.700	.750	.800	.850	.900	.950	.980	1.000	
VALUES	.100E-01	.910	1.22	1.83	2.74	3.05	3.66	4.75	6.09	6.10
.2.2	15.2	16.8	21.3	30.5	34.8	61.0	77.	183.	366.	

Table 6-5. PARAMETERS INCLUDED IN THE UNSATURATED ZONE FLOW DATA GROUP OF EPACML MODEL (concluded)

DATA FOR MATERIAL 1						

VADOSE ZONE FUNCTION VARIABLES						

VARIABLE NAME	UNITS	DISTRIBUTION	PARAMETERS		LIMITS	
			MEAN	STD DEV	MIN	MAX

* Residual water saturation	--	SB	.650E-01	.740E-01	.000E+00	.110
Brook and Corey exponent, EN	--	CONSTANT	.500	.100	.000E+00	1.00
* ALPHA coefficient	--	SB	.700E-01	.171	.000E+00	.250
* BETA coefficient	--	LOG NORMAL	1.89	.155	1.35	3.00

* These values change depending on the underlying unsaturated zone.

using procedures described in U.S. EPA (1990). Thus the values of parameters NP and IMSHGN are ignored. Further, the unsaturated zone is considered to be homogeneous. The value of KPROP = 1 implies that van Genuchten's soil characteristic relationship is to be used.

6.4.2 Material Variables Subgroup

This subgroup includes four variables. The values of the first three--saturated hydraulic conductivity, vadose zone porosity and the air entry pressure head are unsaturated zone soil type dependent. The specific values for three different soils are shown in Table 6-6. The depth of the unsaturated zone was generated using the empirical distribution presented in Table 6-7 and Figure 6-2.

6.4.3 Functional Variables Subgroup

This subgroup includes four variables, all of which are unsaturated zone soil dependent. The specific values used are listed in Table 6-6. Note that since the van Genuchten's relationship for the characteristic curves was selected, the value of Brook and Corey exponent, ENN is neglected by the model.

6.5 UNSATURATED ZONE TRANSPORT DATA GROUP

The unsaturated zone transport data shown in Table 6-8, consists of two subgroups the control parameter subgroup and the vadose transport variables subgroup. The parameters within each group are discussed below.

6.5.1 Control Parameter Subgroup

When the model is run in the steady-state with the depth of the unsaturated zone randomly generated, the variables within this group are ignored by the model. However, default values are printed in the main output file.

Table 6-6. UNSATURATED ZONE FLOW MODEL PARAMETERS FOR DIFFERENT SOIL TYPES

8

Parameters		Limits		Std. Dev.	Min	Max
Variable Name	Units	Distribution ¹	Mean			
<u>SILT LOAM</u>						
Saturated hydraulic conductivity	cm/hr	LOG NORMAL	.343	.989	.000E+00	15.0
Vadose zone porosity	--	CONSTANT	.450	.000E+00	.000E+00	.500
Residual water saturation	--	SB	.680E-01	.710E-01	.000E+00	.110
ALPHA coefficient	--	LOG NORMAL	.190E-01	.120E-01	.000E+00	.150
BETA coefficient	--	SB	1.41	1.63	1.00	2.00
Air entry pressure head	m	CONSTANT	0	--	--	--
<u>SILT CLAY LOAM</u>						
Saturated hydraulic conductivity	cm/hr	SB	.170E-01	2.92	.000E+00	3.50
Vadose zone porosity	--	CONSTANT	.430	.000E+00	.000E+00	.500
Residual water saturation	--	NORMAL	.890E-01	.900E-02	.000E+00	.115
ALPHA coefficient	--	SB	.900E-02	.970E-01	.000E+00	.150
BETA coefficient	--	NORMAL	1.24	.610E-01	1.00	1.50
Air entry pressure head	m	CONSTANT	0	--	--	--
<u>SANDY LOAM</u>						
Saturated hydraulic conductivity	cm/hr	SB	2.30	24.7	.000E+00	30.0
Vadose zone porosity	--	CONSTANT	.410	.000E+00	.000E+00	.500
Residual water saturation	--	SB	.650E-01	.740E-01	.000E+00	.110
ALPHA coefficient	--	SB	.700E-01	.171	.000E+00	.250
BETA coefficient	--	LOG NORMAL	1.89	1.55	1.35	3.00
Air entry pressure head	m	CONSTANT	0	--	--	--

¹ See Section 5.4 for a description of the distributions.

Table 6-7. EMPIRICAL DISTRIBUTION USED TO REPRESENT THE THICKNESS OF THE UNSATURATED ZONE

Serial Number	Cumulative Probability (%)	Depth (m)
1.	0	0.01
2.	5	0.91
3.	10	1.22
4.	20	1.83
5.	25	2.74
6.	30	3.05
7.	35	3.66
8.	40	4.75
9.	45	6.091
10.	50	6.101
11.	60	12.20
12.	65	15.24
13.	70	16.77
14.	75	21.34
15.	80	30.49
16.	85	34.76
17.	90	60.98
18.	95	106.71
19.	98	182.93
20.	100	365.85

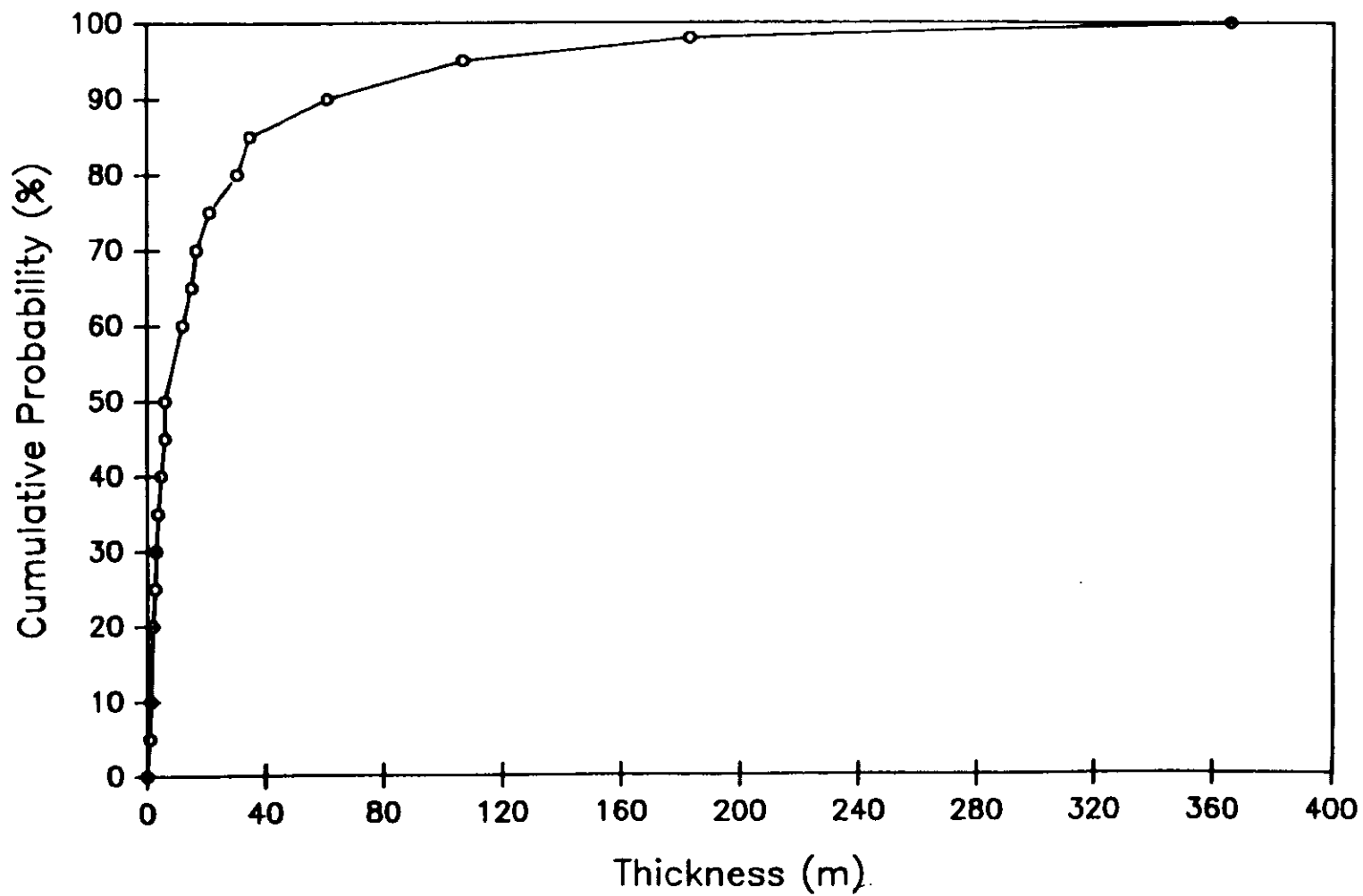


Figure 6--2. Empirical Distribution Used to Represent the Thickness of the Unsaturated Zone

Table 6-8. PARAMETERS INCLUDED IN THE UNSATURATED ZONE TRANSPORT DATA GROUP OF EPACML MODEL

UNSATURATED ZONE TRANSPORT MODEL PARAMETERS

* NLAY	- Number of different layers used	1
* NSTPS	- Number of time values concentration calc	20
* IADV	- Type of transport solution	1
* ISOL	- Type of scheme used in vadose zone	1
* N	- Stehfest terms or number of increments	18
* NTEL	- Points in Lagrangian interpolation	3
* NGPTS	- Number of Gauss points	104
* NIT	- Convolution integral segments	2
* IROUND	- Type of boundary condition	1
* ITSGEN	- Time values generated or input	1
* TMAX	- Max simulation time	-- 10.0
* WTFUN	- Weighting factor	-- 1.2

OPTIONS CHOSEN

 Stehfest numerical inversion algorithm
 Nondecaying continuous source
 Computer generated times for computing concentrations

DATA FOR LAYER 1

VADOSE TRANSPORT VARIABLES

VARIABLE NAME	UNITS	DISTRIBUTION	PARAMETERS		LIMITS	
			MEAN	STD DEV	MIN	MAX
* Thickness of layer	m	CONSTANT	6.10	1.00	.000E+00	500.
Longitudinal dispersivity of layer	m	CONSTANT	.400	.400E-01	.000E+00	10.0
Fractional organic carbon matter	--	SB	.250	7.54	.000E+00	11.0
Bulk density	g/cc	CONSTANT	1.60	.000E+00	.000E+00	2.00
Biological decay coefficient	1/yr	CONSTANT	.000E+00	.200E-01	.000E+00	5.00

* Unsaturated zone transport parameters ignored for steady-state simulations

Thickness of layer set equal to depth of unsaturated zone generated in Monte Carlo mode (Table 6-7)

6.5.2 Vadose Transport Variable Subgroup

This subgroup consists of five parameters shown in Table 6-8. These include the thickness of the unsaturated zone, the longitudinal dispersivity, bulk density, fractional organic carbon matter content, and biological decay coefficient. For contaminant transport computations, the unsaturated zone was simulated as a single layer of thickness equal to the depth of the unsaturated zone generated as part of the unsaturated zone flow data (Section 6.4.2). The longitudinal dispersivity and biological decay coefficient were assigned constant values of 0.40m and 0.00, respectively. Values of the fractional organic carbon matter content and the bulk density are soil dependent. For the three soils used in the simulations, the values are presented in Table 6-9.

6.6 AQUIFER-SPECIFIC DATA

The aquifer-specific input data used in the model are shown in Table 6-10. The specific relationships used to derive porosity (ψ), bulk density (ρ_b), hydraulic conductivity (K), seepage velocity (V_s) and dispersivities have been discussed in detail in Section 4.5.2. The source of each of these data are discussed below.

6.6.1 Temperature

The data used for groundwater temperature are the same as used in the January 16, 1986, Federal Register Notice and are presented in Table 6-10.

6.6.2 Groundwater pH

The groundwater pH distribution has been derived based on an analysis of the STORET data. It is assumed that the groundwater is sufficiently buffered to insure that the pH is not influenced by input of contaminants or changes in temperature.

Table 6-9. VALUES OF BULK DENSITY AND FRACTIONAL ORGANIC CARBON MATTER USED
IN THE UNSATURATED ZONE TRANSPORT MODEL

Variable Name	Units	Distribution ¹	Parameters		Limits	
			Mean	Std.Dev.	Min	Max
<u>SANDY LOAM</u>						
Fractional organic carbon matter	--	SB	.250	7.54	0.0E+0	11.0
Bulk density	g/cc	CONSTANT	1.60	--	--	--
<u>SILTY CLAY LOAM</u>						
Fractional organic carbon matter	--	SB	.26E-01	7.77	0.0E+0	11.0
Bulk density	g/cc	CONSTANT	1.67	--	--	--
<u>SILT LOAM</u>						
Fractional organic carbon matter	--	SB	.39E+01	7.74	0.0E+0	11.0
Bulk density	g/cc	CONSTANT	1.65	--	--	--

¹ See Carsel (1988) 5.3 for a description of the distributions.

Table 6-10. PARAMETERS INCLUDED IN THE AQUIFER-SPECIFIC DATA GROUP OF EPACML MODEL

AQUIFER SPECIFIC VARIABLES										
VARIABLE NAME	UNITS	DISTRIBUTION	PARAMETERS		LIMITS					
			MEAN	STD DEV	MIN	MAX				
Particle diameter	cm	LOG10 UNIFORM	.630E-03	.630E-04	.400E-03	.100				
Aquifer porosity	--	DERIVED	.000E+00	.000E+00	.300	.560				
Bulk density	g/cc	DERIVED	1.64	.000E+00	1.16	1.80				
Aquifer thickness	m	EXPONENTIAL	78.6	78.6	3.00	560.				
Source thickness (mixing zone depth)	m	DERIVED	6.00	.600	2.00	10.0				
Conductivity (hydraulic)	m/yr	DERIVED	.758E+05	.758E+04	31.6	.151E+06				
Gradient (hydraulic)	--	EXPONENTIAL	.309E-01	.310E-01	.100E-04	.100				
Groundwater seepage velocity	m/yr	DERIVED	300.	.000E+00	.100E-01	.925E+04				
Retardation coefficient	--	DERIVED	1.00	.100	1.00	.352E+06				
Longitudinal dispersivity	m	GELHAR	15.2	.700	.100	324.				
Transverse dispersivity	m	RATIO	8.00	.000E+00	.100	41.0				
Vertical dispersivity	m	RATIO	160.	.950E-01	.380	250.				
Temperature of aquifer	C	NORMAL	14.4	5.29	5.00	30.0				
pH	--	NORMAL	6.20	1.28	.300	14.0				
Organic carbon content (fraction)	--	LOG NORMAL	.315E-02	.300E-03	.100E-02	.100E-01				
* Distance to well	m	EMPIRICAL	152.	.000E+00	152.	152.				
Angle off center	degree	CONSTANT	.000E+00	.000E+00	.000E+00	90.0				
Well vertical distance	m	UNIFORM	.000E+00	.500E-01	.000E+00	1.00				
EMPIRICAL CUMULATIVE DISTRIBUTIONS										

Well distance from site for landfill										

PROBABILITIES	.000	.030	.040	.050	.100	.150	.200	.250	.300	.350
.400	.500	.600	.700	.800	.850	.900	.950	.980	1.000	
VALUES	.600	13.7	19.8	45.7	104.	152.	183.	244.	305.	305.
366.	427.	610.	805.	914.	.116E+04	.122E+04	.137E+04	.152E+04	.161E+04	

* Distance to well are different for landfill or surface impoundment scenarios

6.6.3 Fractional Organic Carbon Content

The organic carbon content, f_{OC} , is used to determine the distribution coefficient, K_d . Unfortunately, few if any comprehensive subsurface characterizations of organic carbon content exist. In general the values are low, typically less than .01. A low range for f_{OC} was assumed, and the distribution shape was determined by the distribution of measured dissolved organic carbon recorded as entries to EPA's STORET data base.

6.6.4 Particle-Size Distribution

The data used for the particle-size distribution are the same as used for the January 14, 1986, Federal Register and are presented in Table 6-10.

6.6.5 Hydraulic Gradient

The hydraulic gradient is a function of the local topography, groundwater recharge, volumes and locations and the influence of withdrawals. The probability distribution for the gradient is derived from a survey of RCRA Part B permit applications.

6.6.6 Thickness of the Saturated Zone

The thickness of the saturated zone determines the maximum depth of the plume as it moves downgradient. Literature values taken from measurements and surveys conducted by the Agency were used to derive the distribution for this parameter.

6.6.7 Dispersivities

The longitudinal dispersivity was estimated using Gelhars empirical distribution. The transverse dispersivity was set equal to one-eighth the longitudinal dispersivity, and the vertical dispersivity was set equal to the longitudinal dispersivity divided by 160.

6.6.8 Receptor Well Location-Specific Data

In order to uniquely specify the location of the monitoring point or the receptor well location, the cartesian coordinates need to be specified. As discussed in Section 4.5.4, the x and y coordinates are obtained from values of the radial distance to the well and the angle measured counterclockwise from the plume centerline ($y = 0$). A schematic diagram is shown in Figure 6-3. An empirical distribution was used to estimate the distance to the well. The values are shown in Table 6-11 and Figure 6-4. This is based on a survey by the Agency.

The angle, ψ , is assumed to be uniformly distributed between 0 and 90°. Once x_r and y_r are computed using the trigonometric relations shown in Figure 6-3, y_r is checked to ensure that:

$$y_r \leq \frac{1}{2} (A_w)^{\frac{1}{2}} + (2\alpha_T x_r)^{\frac{1}{2}} \quad (6-2)$$

where:

A_w = area of the facility [m^2]

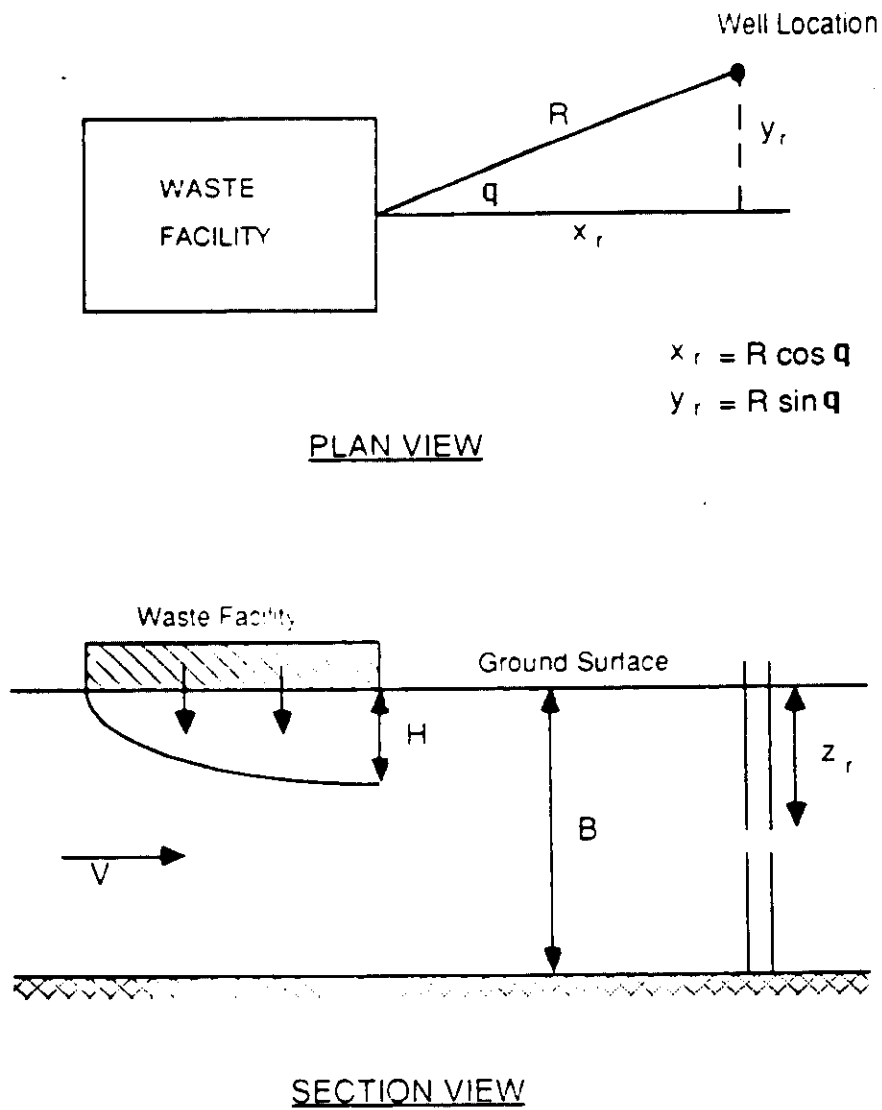
α_T = transverse dispersivity [m]

x_r = x coordinate of the receptor well location [m]

y_r = y coordinate of the receptor well location [m]

The above constraint ensures that the well is randomly located within the approximate width of the contaminant plume.

The depth of the monitoring point is assumed to be uniformly distributed between the top of the saturated zone, $z = 0$, and the bottom, $z = B$.



- Data:
- R follows an empirical distribution (Table 6.9)
 - q uniformly varies between 0° and 90°
 - x_r and y_r constrained to lie within approximate dimensions of the plume
 - z_r uniformly distributed within the saturated zone

Figure 6-3. Schematic of the Well Location

Table 6-11. EMPIRICAL DISTRIBUTION USED TO REPRESENT THE DISTANCE
TO WELL

Cumulative Probability %	Distance to Well (m)
0.0	0.6
3.0	13.7
4.0	19.8
5.0	45.7
10.0	103.6
15.0	152.4
20.0	182.9
25.0	243.8
30.0	304.79
35.0	304.81
40.0	365.7
50.0	426.7
60.0	609.6
70.0	804.6
80.0	914.4
85.0	1158.2
90.0	1219.1
95.0	1371.5
98.0	1523.8
100.0	1609.3

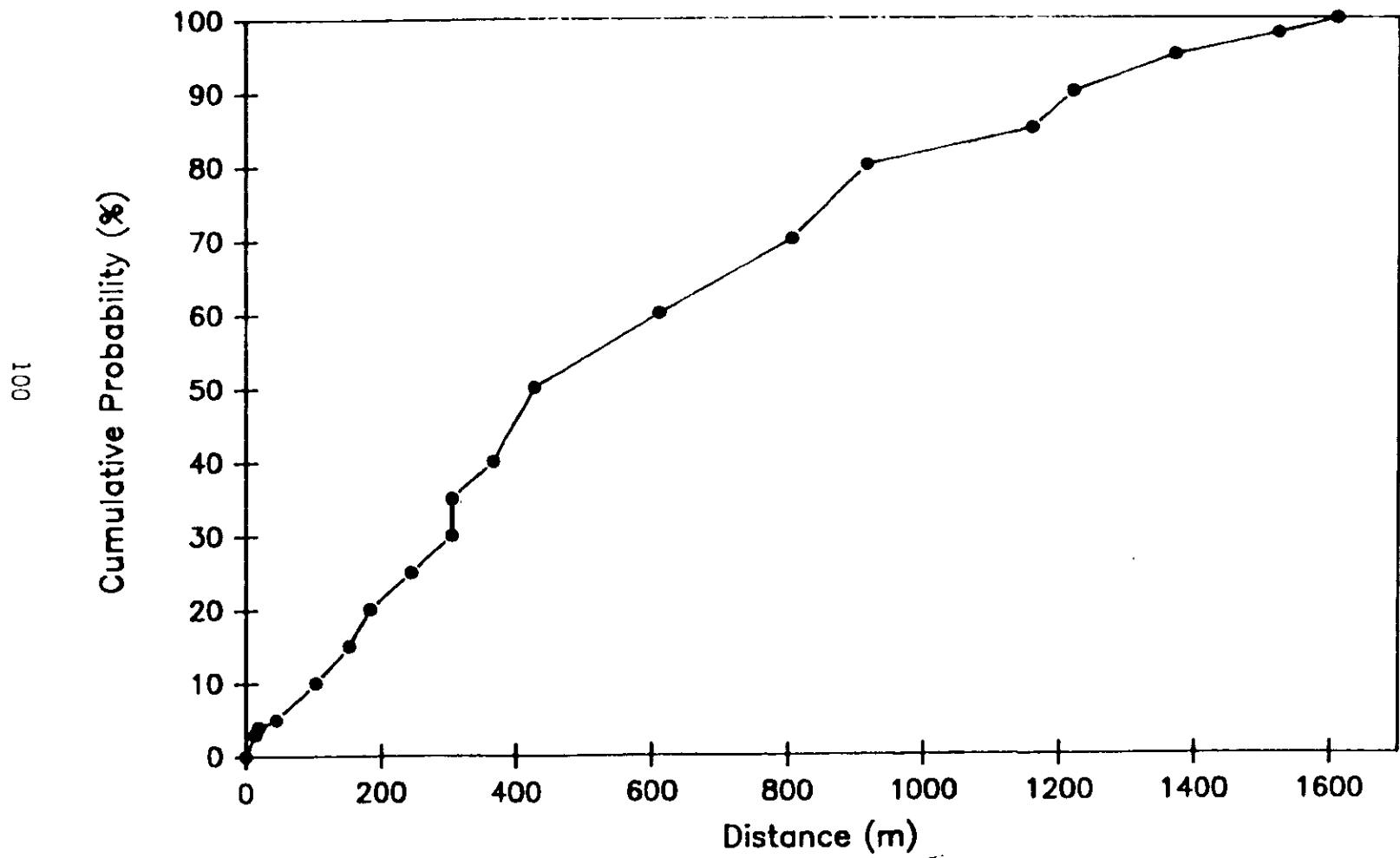


Figure 6-4. Empirical Distribut Used to Represent the Distance to Well

7.1 REFERENCE CASE

A chemical-specific cumulative frequency distribution of the normalized downgradient well concentration that is representative of nationwide uncertainty in the model parameters was developed by running the EPACML model in the Monte Carlo mode. Data used for this was presented in Section 6. The nationwide variation was obtained by dividing the nation into a number of relatively homogeneous environmental settings. Each setting was simulated using EPACML to obtain a cumulative distribution function of the normalized concentration specific for that setting. These individual distributions were combined using weighting factors for the environmental settings (relative nationwide occurrence of each environmental setting) to estimate the composite nationwide distribution based on the total probability theorem. Details of the aggregation procedure are discussed in detail in U.S. EPA (1990).

For the reference case, three different soil types were selected to represent the nationwide variations in the unsaturated zone soil type. Each of these soils was used to represent a soil type underlying a landfill or soil used as the cover material for the landfill. This results in nine different environmental settings. Further, it was assumed that infiltration through the landfill should be less than the ambient recharge (see also EPA 1990). This eliminated three of the nine combinations resulting in six feasible scenarios that are shown in Table 7-1 along with their assigned weights, i.e., their nationwide occurrence.

Table 7-1. WEIGHTS USED TO ESTIMATE THE COMPOSITE NATIONWIDE
DISTRIBUTION OF DAFS FOR LANDFILL SCENARIOS

Soil Type	Cover Soil	Weight %
Sandy Loam	Sandy Loam	2.37
"	Silt Loam	8.72
"	Silty Clay Loam	4.32
Silt Loam	Silt Loam	37.87
"	Silty Clay Loam	18.73
Silty Clay Loam	Silty Clay Loam	28.0

Using the data presented in Section 6 and the six environmental scenarios described above, EPACML simulations were conducted for the reference case. The EPACML model results are in the form of normalized concentrations. These concentrations are the inverse of the Dilution Attenuation Factor (DAF). All the results presented in this chapter are in terms of DAF. Results from the reference case simulations are shown in Table 7-2.

7.2 SENSITIVITY ANALYSIS

EPACML model runs were conducted to test model sensitivity to dispersivity, aquifer temperature, infiltration value, landfill area and well location. Model results were found to be insensitive to aquifer temperature. The two different dispersivity relationships presented in Table 4.3a and b were simulated. Alternative 2 described in Table 4.3b results in generally lower dispersivities and higher DAFs. Model sensitivities to the value of infiltration, well location and landfill area are discussed below.

7.2.1 Infiltration Rate

Contaminant transport in the saturated zone is not a direct function of the infiltration rate. However, as discussed in Section 4.5.1.3, near field dilution (see equations 4-25 and 4-26) is directly proportional to infiltration. Since DAF equals the inverse of normalized concentration, the relationship between infiltration rate and DAF is non-linear. The relationship between infiltration rate and DAF is presented in Figure 7-1.

7.2.2 Location of Well

The method used to determine the location of the well was described in Section 4.5. Briefly, the coordinates of the well location are computed based upon user-specified values of radial distance to the well and the angle ψ , off the plume centerline (the well can be located on either side of the plume centerline). Two different sets of runs were conducted to

Table 7-2. DILUTION/ATTENUATION FACTORS FOR DIFFERENT SCENARIOS FOR REFERENCE CASE

Serial Number	Unsaturated ¹ Zone Soil	Cover Soil for Estimating Infiltration	Percentile ²			
			95	90	85	80
1	Sandy Loam	Sandy Loam	7.63	16.4	42.4	82.6
2	Sandy Loam	Silt Loam	20.7	81.3	193	568
3	Sandy Loam	Silty Clay Loam	17.2	64.5	147	383
4	Silty Clay Loam	Silt Loam	17.9	51.3	159	383
5	Silty Clay Loam	Silty Clay Loam	12.0	45.2	123	311
6	Silt Loam	Silty Clay Loam	12.0	49.8	118	281
	Composite		14.0	51.8	130	325

¹ Also governs the ambient recharge rate.

² Dilution Attenuation Factor is the inverse of the normalized concentration output from EPACML.

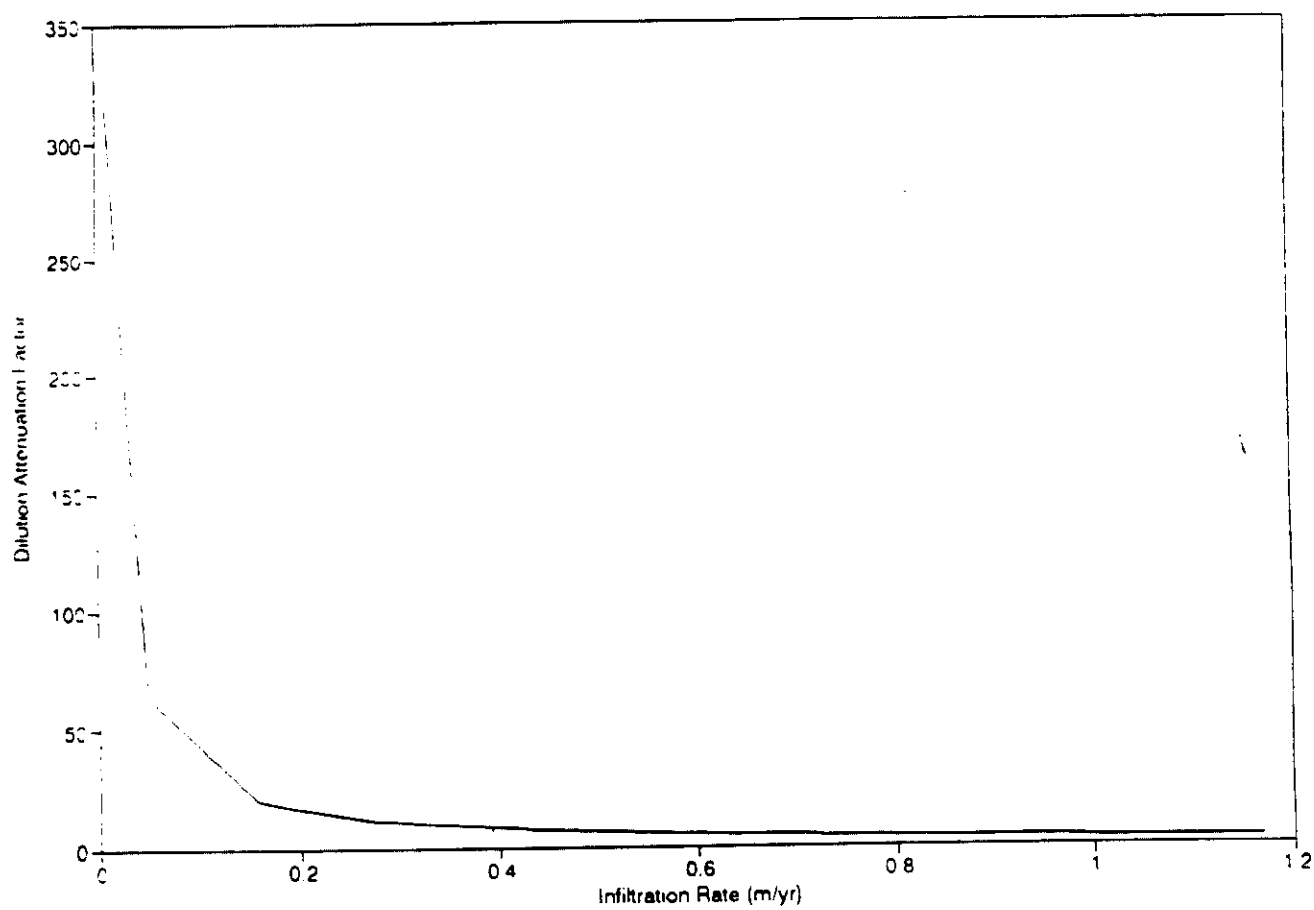


Figure 7-1. Sensitivity of EPACML Results to Infiltration Rate.

test the sensitivity of this method: ψ was restricted to 45 degrees on either side of the centerline (the release case uses 90 degrees), and the restriction that the well location be located within the plume was removed (the reference case restricts the well location to the plume).

Table 7.3 presents a comparison between restricting ψ to 45 degrees and the reference case ($\psi \leq 90$ degrees). Relative to the reference case, restricting ψ to 45 degrees results in a decrease in DAF of approximately 20%. At the 95 percentile value, there is only a 7% decrease, however. At high percentiles the probability that the well is located near the plume centerline increases, resulting in a decrease in the effect of angle restriction.

Table 7-4 shows the effect of not restricting the well location to the plume. If this restriction is removed, there is a large increase in DAF due to the generation of many well locations outside the plume boundary. This effect decreases for high percentiles, since for high percentiles, there is a high probability the well is located near the plume centerline.

7.2.3 Area of Landfill

In EPACML, increasing the area of the landfill increases the mass leaving the landfill. This causes an increase in the down gradient concentration (or decrease in DAF). EPACML was run in deterministic mode for six different areas. Table 7-5 and Figure 7-2 present the results from these simulations. The results indicate that there is a non-linear relationship between DAF and area as indicated by the approximate straight line fit to the data on Figure 7-2 (which has log-log scales). Area affects the downgradient concentrations in two ways, an increase in area results in an increase in near field dilution (see equation 4-26) and an increase in the spread of the gaussian source (Section 4.5.1.2).

Table 7-3. EFFECT ON DAF OF RESTRICTING ANGLE OFF PLUME CENTERLINE TO 45 DEGREES (well restricted to plume)

	80	Percentiles 85	90	95
45 degrees	264	104	40.6	13.0
90 degrees	325	130	51.8	14.0

Table 7-4. EFFECT ON DAF OF NOT RESTRICTING WELL TO PLUME

	80	Percentiles 85	90	95
Not Restricted	8280	1580	239.	35.4
Restricted	325	130	51.8	14.0
% Change	2450	1115	361.	152.

Table 7-5. EFFECT ON DAF OF CHANGING AREA OF LANDFILL

Area (Acres)	Percentiles			
	80	85	90	95
4	1430	709	223	67.1
12	757.	332	148	34.6
40	323	136	51.8	15.0
122	149	56.8	23.9	7.58
280	77.5	35.5	14.5	4.85
5250	13.5	7.81	4.44	2.14

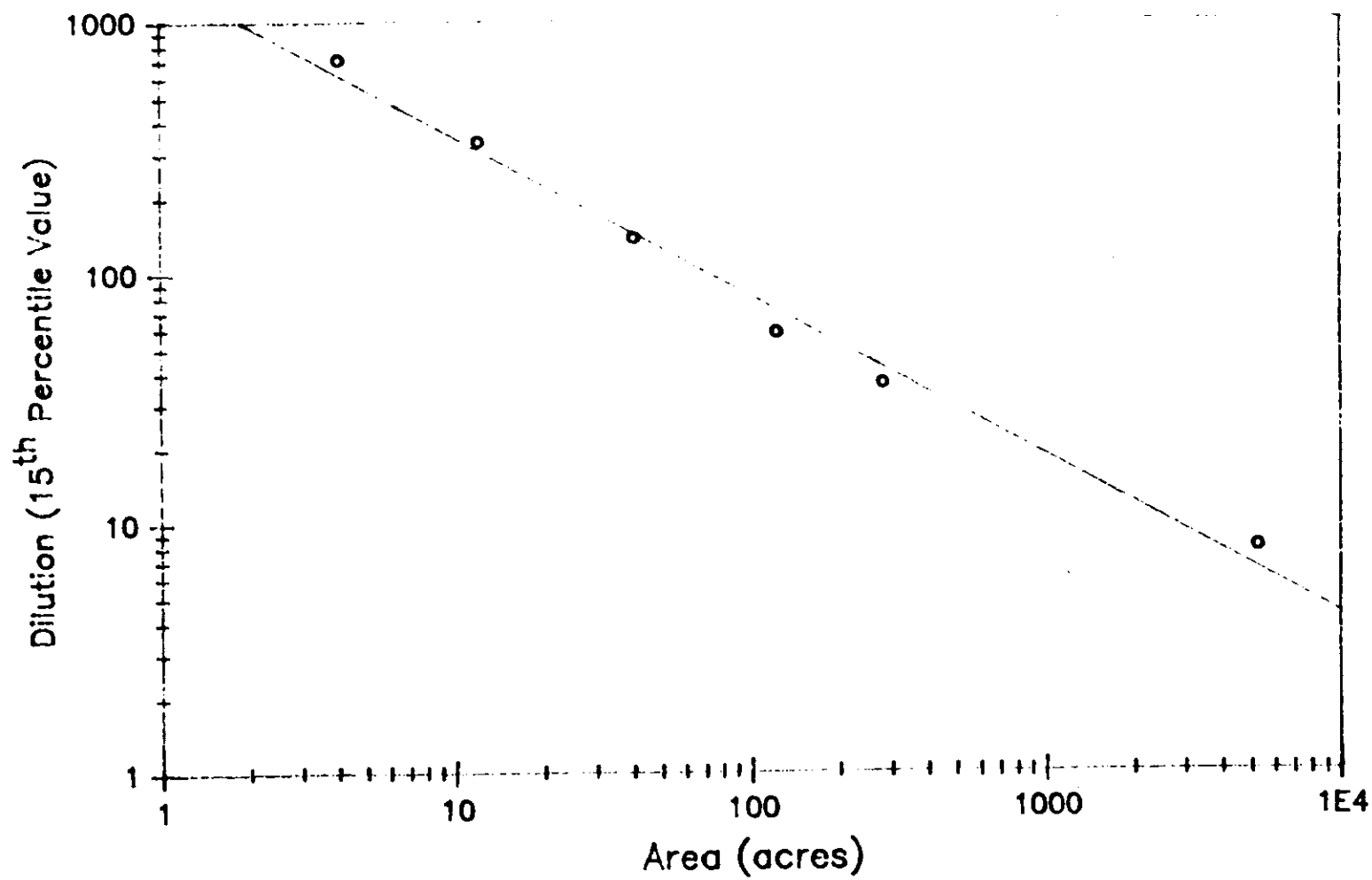


Figure 7-2. Dilution Attenuation Factor as a Function of Area of Landfill

NOTATION

- A_w = Area of land disposal unit [m^2]
- B = Thickness of the saturated zone [m]
- C = Concentration of the contaminant [mg/l]
- C_1 = Concentration of the contaminant in the leachate from the waste facility or the bottom of the unsaturated zone [mg/l]
- C_0 = Maximum gaussian-source concentration [mg/l]
- C_T = Health based threshold concentration [mg/l]
- d = Representative particle size for the porous media [cm]
- D_v = The longitudinal dispersion coefficient in the unsaturated zone [m^2/yr]
- D_x, D_y, D_z = Hydrodynamic dispersion coefficient in the x, y and z directions in saturated zone [m^2/yr]
- D_x^*, D_y^*, D_z^* = Retarded hydrodynamic dispersion coefficient in the x, y and z directions in the saturated zone [m^2/yr]
- E_a = Arrhenius activation energy [kcal/mole]
- f_{oc} = Percent organic carbon in the saturated zone [g/g]
- f_{om} = Percent organic matter content [dimensionless]
- $F_C(C'_w)$ = Nationwide Composite Cumulative probability distribution function for normalized downgradient well concentration
- H = Thickness of source within the saturated zone [m]
- I_f = Infiltration rate through the land disposal facility [m/yr]
- k_{rw} = The relative hydraulic conductivity [dimensionless]
- K = Hydraulic conductivity for the saturated zone [m/yr]
- K_d = Distribution coefficient for chemical in the liquid and solid phase [cc/g]
- K_{dv} = The contaminant distribution coefficient for the unsaturated zone [cc/g]

K_{OC} = Normalized distribution coefficient for organic carbon [μ/g]
 K_V = The saturated hydraulic conductivity [m/yr]
 z = The thickness of a layer
 L = Dimension of the waste facility parallel to the direction of ground water flow [m]
 L_V = The thickness of the unsaturated zone [m]
 M_a = Mass entering the saturated zone due to advection [kg/yr]
 M_d = Mass entering the saturated zone due to dispersion [kg/yr]
 M_L = Mass leaching out of the facility [kg/yr]
 M_T = Total mass, sum of advective and dispersive, entering the saturated zone [kg/yr]
 n = The number of homogenous layers within the unsaturated zone [dimensionless]
 P_I = Probability of occurrence of hydrogeologic setting I
 q = Infiltration into the contaminant plume outside the waste facility [m/yr]
 R_g = Universal gas constant [1.987E-3 Kcal/°C-mole]
 R_s = Retardation factor for the saturated zone [dimensionless]
 R_V = The unsaturated zone retardation factor [dimensionless]
 $s(t-T)$ = The unit step function with a value of unity for $t > T$ and zero for $t < T$ [t and T are in years]
 S_e = The effective saturation [dimensionless]
 S_w = The fractional saturation within the unsaturated zone [cc/cc]
 S_{wr} = The residual water saturation [dimensionless]
 t = Elapsed time [yr]
 T = Temperature of the saturated zone [°C]
 T_s = Duration of pulse source [yr]
 V_s = Seepage velocity in the saturated zone [m/yr]

V_s^* = Retarded seepage velocity in the saturated zone [m/yr]
 V_v = The steady-state unsaturated zone seepage velocity [m/yr]
 W = Dimension of the waste facility orthogonal to the direction of groundwater flow [m]
 x_r = x coordinate of the receptor well [m]
 x = Longitudinal coordinate direction [m]
 y = Lateral coordinate direction [m]
 y_r = y coordinate of the receptor well [m]
 z = Vertical coordinate pointing downwards [m]
 z_r = z coordinate of the receptor well [m]
 α = Soil-specific parameter [1/m]
 α' = Acid-catalysis hydrolysis rate enhancement factor for sorbed phase [dimensionless]
 α_L = Longitudinal (x-direction) dispersivity [m]
 α_T = Transverse (y-direction) dispersivity [m]
 α_v = The longitudinal dispersivity [m]
 α_V = Vertical (z-direction) dispersivity [m]
 $\beta_{s,v}$ = Soil-specific parameters [dimensionless]
 θ = Effective porosity of the saturated zone [dimensionless]
 λ_b = Biological decay coefficient for the chemical in the saturated zone [1/yr]
 λ_s = Overall decay coefficient within the saturated zone [1/yr]
 λ_v = The first-order degradation rate within the unsaturated zone [1/yr]
 λ_1 = Liquid-phase chemical decay coefficient [1/yr]
 λ_2 = Solid-phase chemical decay coefficient [1/yr]
 Λ = The source concentration decay rate [1/yr]

- ρ_b = Bulk density of the saturated soil [g/cc]
- ρ_{bv} = The bulk density of the unsaturated zone [g/cc]
- σ = Standard deviation of the gaussian contaminant source [m]
- ψ = The pressure head [m]
- $\bar{\psi}$ = The representative pressure head for the soil layer between z and $z - \Delta z$
- ψ_a = The air entry pressure head, which is subsequently assumed zero [m]
- φ = Angle measured clockwise between well location and the x axis (degrees)
- ω = A weighting coefficient ($0 \leq \omega \leq 1$).

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APPENDIX A
DERIVATION OF THE ADVECTIVE AND DISPERSIVE
FLUX EMANATING INTO THE AQUIFER AT THE
SOURCE $x = 0$ FOR STEADY-STATE CONDITIONS

Deviation of the Advective and Dispersive Flux Emanating into the Aquifer at the Source $x = 0$ for Steady-State Conditions

The steady-state concentration can be expressed as:

$$C^*(x, y, z) = \frac{H}{B} C_f^*(x, y) + \Delta C_p^*(x, y, z) \quad (A.1)$$

where C_f^* and ΔC_p^* are functions given by

$$C_f^*(x, y) = \hat{\xi} \sqrt{\beta_0} \int_{v=-\infty}^{\infty} F^*(x, y, v, \beta_0) dv \quad (A.2)$$

$$\Delta C_p^*(x, y, z) = \frac{2\hat{\xi}}{\pi} \sum_{n=1}^{\infty} \frac{1}{n} \cos\left(\frac{n\pi z}{B}\right) \sin\left(\frac{n\pi H}{B}\right) \sqrt{\beta_n} \int_{v=-\infty}^{\infty} F^*(x, y, v, \beta_n) dv \quad (A.3)$$

in which

$$F^*(x, y, v, \beta_n) = K_1\left(\sqrt{\beta_n \left(\frac{x^2}{D_x^*} + \frac{v^2}{D_y^*}\right)}\right) \exp\left(-\frac{vy}{\sigma^2} - \frac{y^2}{2\sigma^2}\right) \frac{1}{\sqrt{\left(\frac{x^2}{D_x^*} + \frac{v^2}{D_y^*}\right)}} \quad n=0, 1, \dots \quad (A.4)$$

$$\hat{\xi} = \frac{C_0 x}{\pi \sqrt{D_x^* D_y^*}} \exp\left(\frac{V_s^* x}{2D_x^*} - \frac{y^2}{2\sigma^2}\right) \quad (A.5)$$

$$\beta_0 = \frac{V_s^{*2}}{4D_x^*} + \lambda \quad (A.6)$$

$$\beta_n = \beta_0 + \frac{n^2 \pi^2}{B^2} D_z^* \quad (A.7)$$

where $K_1(\cdot)$ is a modified Bessel function of the second kind. The above equations are the steady-state solution to the partial differential equation given by Eq. 4.1 and boundary conditions given by Eq. 4.4

The following relationship is given on page 482, #3.914 of Gradshteyn and Ryzh (1965) for the K_1 Bessel function.

$$\int_{-\infty}^{\infty} K_1 \left(\sqrt{\beta_n \left(\frac{x^2}{D_x^*} + \frac{v^2}{D_y^*} \right)} \right) \frac{1}{\sqrt{\left(\frac{x^2}{D_x^*} + \frac{v^2}{D_y^*} \right)}} = \frac{1}{x} \sqrt{\frac{D_x^* D_y^*}{\beta_n}} \int_{u=0}^{\infty} \cos(uv) \exp \left(-x \sqrt{\frac{u^2 D_y^*}{D_x^*} + \frac{\beta_n}{D_x^*}} \right) du \quad (A.8)$$

For the special case of $y=0$ and $z=0$, the integral of $F^*(x,0,v,\beta_n)$ with respect to v can be performed with the aid of Eq. A.8.

$$\int_{v=-\infty}^{\infty} F^*(x,0,v,\beta_n) dv = \frac{1}{x} \sqrt{\frac{D_x^* D_y^*}{\beta_n}} \int_{u=0}^{\infty} \exp \left(-x \sqrt{\frac{u^2 D_y^*}{D_x^*} + \frac{\beta_n}{D_x^*}} \right) \cdot \int_{v=-\infty}^{\infty} \cos(uv) \exp \left(-\frac{v^2}{2\sigma^2} \right) dv du \quad (A.9)$$

The last right hand side integral of Eq. A.9 can be evaluated as follows

$$\int_{v=-\infty}^{\infty} \cos(uv) \exp \left(-\frac{v^2}{2\sigma^2} \right) dv = \sigma \sqrt{2\pi} \exp \left(-\frac{u^2 \sigma^2}{2} \right) \quad (A.10)$$

Substitute Eq. A.10 into Eq. A.9

$$\int_{v=-\infty}^{\infty} F^*(x,0,v,\beta_n) dv = \frac{\sigma}{x} \sqrt{\frac{2\pi D_x^* D_y^*}{\beta_n}} \int_{u=0}^{\infty} \exp \left[-\frac{u^2 \sigma^2}{2} - x \sqrt{\frac{u^2 D_y^*}{D_x^*} + \frac{\beta_n}{D_x^*}} \right] du \quad (A.11)$$

Substitution of Eq. A.11 into Eqs. A.2 and A.3 will yield the solution shown by Eqs. 4.12a and 4.12b.

$$C_f^*(x,0) = \xi^* \int_{u=0}^{\infty} \exp \left[-\frac{u^2 \sigma^2}{2} - x \sqrt{\frac{u^2 D_y^*}{D_x^*} + \frac{\beta_0}{D_x^*}} \right] du \quad (A.12)$$

A-3

$$\Delta C_p^*(x,0,0) = \frac{2\xi^*}{\pi} \sum_{n=1}^{\infty} \frac{1}{n} \sin\left(\frac{n\pi H}{B}\right) \int_{u=0}^{\infty} \exp\left[-\frac{u^2 \sigma^2}{2} - x \sqrt{\frac{u^2 D_y^*}{D_x^*} + \frac{B_n}{D_x^*}}\right] du \quad (A.13)$$

where

$$\xi^* = \frac{2C_0 \sigma}{\sqrt{2\pi}} \exp\left(\frac{V_s^* x}{2D_x^*}\right) \quad (A.14)$$

and where B_0 and B_n are given by Eqs. A.6 and A.7.

At any point in the aquifer, the total mass flux density along the x axis is defined as the sum of advected mass flux and dispersive mass flux densities [kg/(yr m²)].

$$\text{flux density} = \theta V_s^* C^*(x,y,z) - \theta D_x \frac{\partial C^*}{\partial x}(x,y,z) \quad (A.15)$$

In order to compute the total mass flux \dot{m}_g [kg/yr], the flux density is integrated over a specified cross-sectional area. Since we are interested in measuring the total mass flux that enters the aquifer along the x axis at the x=0 boundary, the flux density is integrated over the saturated depth of the aquifer B and over the infinite y axis plane. Hence

$$\dot{m}_g = \theta \int_{y=-\infty}^{\infty} \int_{z=0}^B (\text{flux density}) dy dz \quad \text{at } x = 0 \quad (A.16)$$

where θ is the porosity [cc/cc].

Substitute Eq. A.15 into Eq. A.16

$$\dot{m}_g = \theta V_s^* \int_{y=-\infty}^{\infty} \int_{z=0}^B C^*(0,y,z) dy dz - \theta D_x \int_{y=-\infty}^{\infty} \int_{z=0}^B \frac{\partial C^*}{\partial x}(0,y,z) dy dz \quad (A.17)$$

Substitute Eq. A.1, A.2 and A.3 into Eq. A.17. The integration over the y variable in $C^*(x,y,z)$ will be performed first.

$$\int_{y=-\infty}^{\infty} C^*(x,y,z) dy = \frac{H}{B} \int_{y=-\infty}^{\infty} C_f^*(x,y) dy + \int_{y=-\infty}^{\infty} \Delta C_p^*(x,y,z) dy \quad (A.)$$

Note the integrations of Eq. A.18 will be first done with the variable x not set equal to zero. The variable x can only be set to zero after the x derivative of Eq. A.18 is performed.

The only term in C_f^* and ΔC_p^* that contains a y variable in Eqs. A.2 and A.3 is that of $\hat{\xi} F^*(x,y,v,\beta_n)$. Then

$$\int_{y=-\infty}^{\infty} \hat{\xi} F^*(x,y,v,\beta_n) dy = \frac{C_0}{\pi_0} \frac{x}{\sqrt{D_x^* D_y^*}} \exp\left(\frac{V_s^* x}{2D_x^*} - \left(\frac{v^2}{2\sigma^2}\right)\right) K_1\left(\sqrt{\beta_n \left(\frac{x^2}{D_x^*} + \frac{y^2}{D_y^*}\right)}\right) \cdot \sqrt{\left(\frac{x^2}{D_x^*} + \frac{y^2}{D_y^*}\right)} \int_{y=-\infty}^{\infty} \exp\left(\frac{-vy}{\sigma^2} - \frac{y^2}{2\sigma^2}\right) dy \quad (A.19)$$

The right hand side integral of Eq. A.19 can be solved as

$$\int_{y=-\infty}^{\infty} \exp\left(\frac{-vy}{\sigma^2} - \frac{y^2}{2\sigma^2}\right) dy = \sigma\sqrt{2\pi} \exp\left(\frac{v^2}{2\sigma^2}\right) \quad (A.20)$$

Substitute Eqs. A.19 and A.20 into the integral of C_f^*

$$\int_{y=-\infty}^{\infty} C_f^*(x,y) dy = C_0 x \sigma \sqrt{\frac{2B_0}{\pi D_x^* D_y^*}} \exp\left(\frac{V_s^* x}{2D_x^*}\right) \int_{v=-\infty}^{\infty} \frac{K_1\left(\sqrt{B_0 \left(\frac{x^2}{D_x^*} + \frac{v^2}{D_y^*}\right)}\right)}{\sqrt{\left(\frac{x^2}{D_x^*} + \frac{v^2}{D_y^*}\right)}} dv \quad (A.21)$$

and the integral of ΔC_p^*

$$\int_{y=-\infty}^{\infty} \Delta C_p^*(x,y,z) dy = \frac{C_0 x}{2\pi} \sigma \sqrt{\frac{2}{\pi D_x^* D_y^*}} \exp\left(\frac{V_s^* x}{2D_x^*}\right) \sum_{n=1}^{\infty} \frac{1}{n} \cos\left(\frac{n\pi z}{B}\right) \sin\left(\frac{n\pi H}{B}\right) \cdot$$

$$\sqrt{B_n} \int_{v=-\infty}^{\infty} \frac{K_1\left(\sqrt{B_n \left(\frac{x^2}{D_x^*} + \frac{v^2}{D_y^*}\right)}\right)}{\sqrt{\frac{x^2}{D_x^*} + \frac{v^2}{D_y^*}}} dv \quad (A.22)$$

The right hand side integrals of Eqs. A.21 and A.22 can be evaluated (p.705, # 6.596.3; Gradshteyn and Ryzhik, 1965).

$$\int_{y=-\infty}^{\infty} \frac{K_1 \left(\sqrt{B_n \left(\frac{x^2}{D_x^*} + \frac{y^2}{D_y^*} \right)} \right)}{\sqrt{\frac{x^2}{D_x^*} + \frac{y^2}{D_y^*}}} dy = \frac{\pi}{x} \sqrt{\frac{D_x^* D_y^*}{B_n}} \exp\left(-x \sqrt{\frac{B_n}{D_x^*}}\right) \quad n=0,1,\dots \quad (A.23)$$

Substitute the solution of Eq. A.23 into Eq. A.21 and A.22

$$\int_{y=-\infty}^{\infty} C_f^*(x,y) dy = C_0 \sigma \sqrt{2\pi} \exp\left(\frac{V_s^* x}{2D_x^*} - x \sqrt{\frac{B_0}{D_x^*}}\right) \quad (A.24)$$

$$\int_{y=-\infty}^{\infty} \Delta C_p^*(x,y,z) dy = C_0 2\sigma \sqrt{\frac{2}{\pi}} \sum_{n=1}^{\infty} \frac{1}{n} \cos\left(\frac{n\pi z}{B}\right) \sin\left(\frac{n\pi H}{B}\right) \exp\left(\frac{V_s^* x}{2D_x^*} - x \sqrt{\frac{B_n}{D_x^*}}\right) \quad (A.25)$$

In order to evaluate the dispersive flux, we will need to evaluate the y integral of the x derivatives of C_f^* and ΔC_p^* . Differentiate Eqs. A.24 and A.25 with respect to x

$$\int_{y=-\infty}^{\infty} \frac{\partial C_f^*(x,y)}{\partial x} dy = C_0 \sigma \sqrt{2\pi} \left(\frac{V_s^*}{2D_x^*} - \sqrt{\frac{B_0}{D_x^*}} \right) \exp\left(\frac{V_s^* x}{2D_x^*} - x \sqrt{\frac{B_0}{D_x^*}}\right) \quad (A.26)$$

$$\int_{y=-\infty}^{\infty} \frac{\partial \Delta C_p^*(x,y,z)}{\partial x} dy = C_0 2\sigma \sqrt{\frac{2}{\pi}} \sum_{n=1}^{\infty} \frac{1}{n} \cos\left(\frac{n\pi z}{B}\right) \sin\left(\frac{n\pi H}{B}\right) \left(\frac{V_s^*}{2D_x^*} - \sqrt{\frac{B_n}{D_x^*}} \right) \exp\left(\frac{V_s^* x}{2D_x^*} - x \sqrt{\frac{B_n}{D_x^*}}\right) \quad (A.27)$$

Integrate Eqs. A.24 to A.27 with respect to the z variable between 0 and B

$$\int_{z=0}^B \int_{y=-\infty}^{\infty} C_f^*(x,y) dy dz = C_0 \sigma \sqrt{2\pi} B \exp\left(\frac{V_s^* x}{2D_x^*} - x \sqrt{\frac{B_0}{D_x^*}}\right) \quad (A.28)$$

$$\int_{z=0}^B \int_{y=-\infty}^{\infty} \Delta C_p^*(x,y,z) dy dz = 0 \quad (A.29)$$

$$\int_{z=0}^B \int_{y=-\infty}^{\infty} \frac{\partial C_f^*(x,y)}{\partial x} dy dz = C_0 \alpha \sqrt{2\pi} B \left(\frac{V_s^*}{2D_x^*} - \sqrt{\frac{B_0}{D_x^*}} \right) \exp\left(\frac{V_s^* x}{2D_x^*} - x \sqrt{\frac{B_0}{D_x^*}}\right) \quad (A.30)$$

$$\int_{z=0}^B \int_{y=-\infty}^{\infty} \frac{\partial \Delta C_p^*(x,y,z)}{\partial x} dy dz = 0 \quad (A.31)$$

The infinite series of Eqs. A.25 and A.27 vanish when integrated with respect to z since the integral of $\cos(n\pi z/B)$ is a sine function which vanishes at the limits 0 and B .

Evaluate the integral solutions of Equations A.28 to A.31 at $x=0$ and substitute into Eq. A.17 in order to compute the total mass flux

$$\dot{m}_g = \theta V_s^* \frac{H}{B} C_0 \alpha \sqrt{2\pi} B - \theta D_x^* \frac{H}{B} C_0 \alpha \sqrt{2\pi} B \left(\frac{V_s^*}{2D_x^*} - \sqrt{\frac{B_0}{D_x^*}} \right) \quad (A.32)$$

where

$$V_s^* = V_s^1 / R_s$$

$$D_x^* = D_x^1 / R_s$$

Substitute β_0 from Eq. A.6 into Eq. A.32 and rearrange to get the final solution for the total steady state mass flux \dot{m}_g [kg/yr].

$$\dot{m}_g = H \sqrt{2\pi} V_s^1 \theta \alpha C_0 (1 + m_{df}) \quad (A.33)$$

The first term of Eq. A.33 represents the contribution of advective flux and the second term m_{df} is the fractional increase in the steady state mass flux due to the contribution of dispersive flux.

$$m_{df} = -\frac{1}{2} + \frac{1}{2} \sqrt{1 + \frac{\lambda 4 D_x^*}{V_s^{*2}} x} \quad (A.34)$$

Note that the factor m_{df} is equal to zero in the event that the dispersive flux is neglected or if there is no decay.

Reference

Gradshteyn, I.S. and I.M. Ryzhik. 1965. Table of Integrals, Series and Products. Academic Press, New York. 1086 pages.

APPENDIX B
SIMPLIFIED ESTIMATION FOR DEPTH OF PENETRATION

Simplified Estimation for Depth of Penetration

The depth of penetration of a solute plume that is developing under a surface impoundment can be estimated by separating the contribution of advection and dispersion during solute transport

$$H = h_{adv} + h_{disp} \quad (1)$$

where H [L] is the depth of penetration, h_{adv} [L] is the vertically advected component of the penetration depth and h_{disp} [L] is the vertically dispersed component of the penetration depth.

The advected depth h_{adv} is the depth that a particle would be transported under the influence of vertical advection

$$h_{adv} = \int_{t=0}^{\tau} V_z dt \quad (2)$$

where V_z [L/T] is the vertical seepage velocity and τ [T] is time of travel. If the vertical seepage velocity is a constant with depth, then

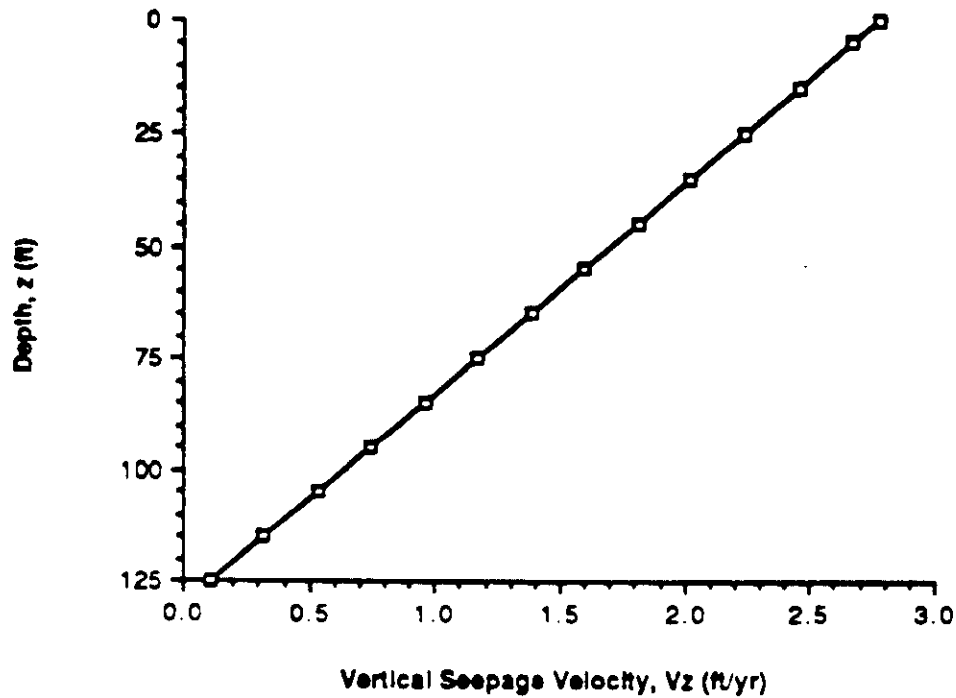
$$h_{adv} = V_z \tau \quad (3)$$

However, under impoundments, the vertical seepage velocity varies linearly with depth, with a maximum value at the top of the water table and zero at the bottom of the aquifer. A numerical solution for a surface impoundment was performed using SEFTRAN, with the vertical velocity variation under the impoundment plotted in Figure 1. This variation can be modeled mathematically as

$$V_z = V_{z0}(1-z/B) \quad (4)$$

where B [L] is the saturated aquifer thickness, z [L] is the depth from the top of the water table and V_{z0} [L/T] is the maximum vertical seepage velocity. V_{z0} can be estimated from the net vertical recharge rate.

Figure 1. Variation in the vertical seepage velocity with depth



SEFTRAN DATA

$I = 10$ in/yr	Net recharge rate
$p = 0.3$	porosity
$H_0 = 132.5$ ft	upstream water table elevation
$H_L = 118.0$ ft	downstream water table elevation
$L = 8000$ ft	distance between boundaries
$K_x = 36500$ ft/yr	horizontal hydraulic conductivity
$K_z = 3650$ ft/yr	vertical hydraulic conductivity
$\Delta x = 200$ ft	horizontal element size
$\Delta z = 10$ ft	vertical element size
t	steady state

As written, Eq. 2 cannot be integrated since V_z is not an explicit function of time. Consider the following differential equation for the vertical seepage velocity

$$\frac{dz}{dt} = V_z(z) \quad (5)$$

Rearrange terms in Eq. 5 and integrate to depth h_{adv}

$$\int_{z=0}^{h_{adv}} \frac{dz}{V_z(z)} = \int_{t=0}^{\tau} dt \quad (6)$$

Substitute Eq. 4 into Eq. 6 and integrate to get

$$\frac{-B}{V_{z0}} \ln(1 - h_{adv}/B) = \tau \quad (7)$$

Solve for h_{adv} from Eq. 7

$$h_{adv} = B \left(1 - e^{\frac{-V_{z0}\tau}{B}} \right) \quad (8)$$

The time of travel τ [T] can be estimated as the time it takes for a particle to be advected horizontally under an impoundment of length L [L]

$$\tau = \frac{L}{V_x} \quad (9)$$

where V_x [L/T] is the horizontal seepage velocity. V_x is assumed to be a constant.

Prickett, Naymik and Lonnquist (1981) estimate the magnitude of the effect of dispersion on particle transport as

$$\Delta_{long} = \sqrt{2\alpha_L V \tau} \quad (10)$$

$$\Delta_{vert} = \sqrt{2\alpha_v V \tau} \quad (11)$$

where α_L and α_V [L] are the longitudinal and vertical dispersivities; V [L/T] is the magnitude of the seepage velocity; and Δ_{long} and Δ_{vert} [L] are the longitudinal and vertical dispersed distances that correspond to one standard deviation of random transport. If the effect of the horizontal seepage velocity is assumed to be much larger than that of the vertical, then the dispersed depth is estimated from Eq. 11 as

$$h_{disp} = \sqrt{2\alpha_V V_x \tau} \quad (12)$$

Hence, the total depth of penetration is the sum of the vertically advected and dispersed components. Substitute Eqs. 8 and 12 into Eq. 1 to obtain the total estimated depth of penetration

$$H = B \left(1 - e^{\frac{-V_{z0}\tau}{B}} \right) + \sqrt{2\alpha_V V_x \tau} \quad (13)$$

The solution to Eq. 13 needs to be checked when evaluating any particular case so that a value of H greater than the aquifer thickness B is not used. If the computed H is greater than B , set H equal to B .

References

Prickett, T., T. Naymik and C. Lonquist. 1981. A random-walk solute transport model for selected groundwater quality evaluations. Bulletin 65 Illinois State Water Survey, Department of Energy and Natural Resources, Champaign, Illinois. 103 pages.